Class 6: R Functions

Kendall Lin

1/23/2020

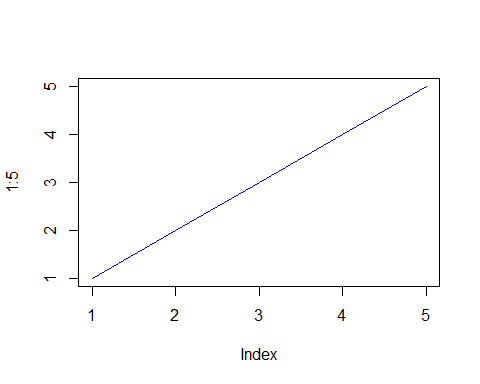
# Functions

## Level 2 heading

### Level 3 heading

read.table(“Your File Name”, Header = True, sep = ’)

plot(1:5, typ = "l", col = "blue")



Lets see more about file import(i.e. reading files into R). The main read function in base R is read.table()

t1 <- read.table("test1.txt")

We need to add arguments to get this file imported

t1<- read.table("test1.txt", header = T, sep = ",")

Or we could just use read.csv() which as the arguments I want in this case!

t1<- read.csv("test1.txt")

t2<- read.table("test2.txt", sep= "$", header = T)

t3 <- read.table("test3.txt")

#Back to functions Out first example function:

add <- function(x, y = 1){  
 #Sum the input x and y  
 x+y  
}

Works with vectors too

add(c(1,2,3),c(1,2,9))

## [1] 2 4 12

What is this range() function?

x<- c(1,3,4,11)  
range(x)

## [1] 1 11

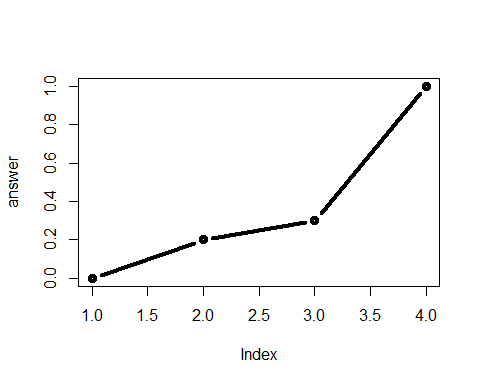
rescale <- function(x) {  
 rng <-range(x, na.rm = T)  
 (x - rng[1]) / (rng[2] - rng[1])  
}  
rescale(c(1,2,NA,3, 10))

## [1] 0.0000000 0.1111111 NA 0.2222222 1.0000000

rescale3<- function(x, na.rm=TRUE, plot=FALSE) {  
   
 rng <-range(x, na.rm=na.rm)  
 print("Hello")  
   
 answer <- (x - rng[1]) / (rng[2] - rng[1])  
   
 print("is it me you are looking for?")  
   
 if(plot) {  
 plot(answer, typ="b", lwd=4)  
 }  
 print("I can see it in ...")  
 return(answer)  
}

rescale3(x, plot = T)

## [1] "Hello"  
## [1] "is it me you are looking for?"



## [1] "I can see it in ..."

## [1] 0.0 0.2 0.3 1.0

library(bio3d)

Hands on Section B.

library(bio3d)  
s1 <- read.pdb("4AKE") # kinase with drug

## Note: Accessing on-line PDB file

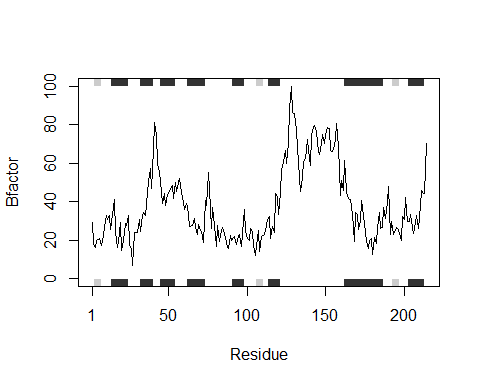
s2 <- read.pdb("1AKE") # kinase no drug

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

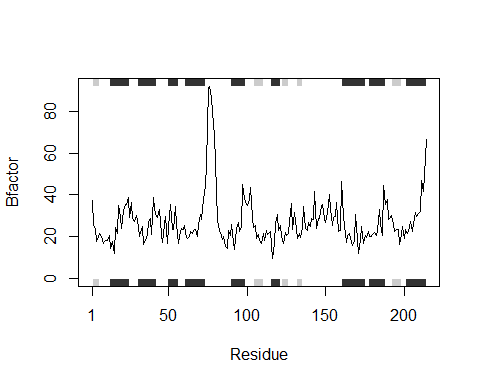
s3 <- read.pdb("1E4Y") # kinase with drug

## Note: Accessing on-line PDB file

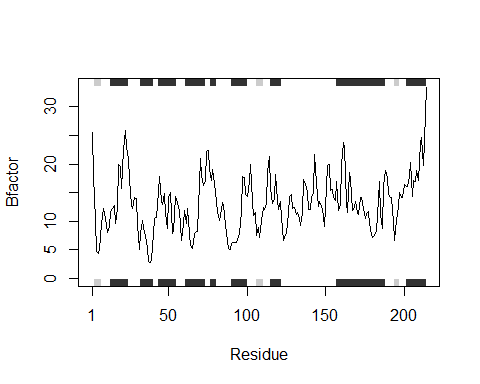
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")  
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")  
s3.chainA <- trim.pdb(s3, chain="A", elety="CA")  
  
s1.b <- s1.chainA$atom$b  
s2.b <- s2.chainA$atom$b  
s3.b <- s3.chainA$atom$b  
  
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")



plotb3(s2.b, sse=s2.chainA, typ="l", ylab="Bfactor")



plotb3(s3.b, sse=s3.chainA, typ="l", ylab="Bfactor")



class(s1)

## [1] "pdb" "sse"

str(s1)

## List of 8  
## $ atom :'data.frame': 3459 obs. of 16 variables:  
## ..$ type : chr [1:3459] "ATOM" "ATOM" "ATOM" "ATOM" ...  
## ..$ eleno : int [1:3459] 1 2 3 4 5 6 7 8 9 10 ...  
## ..$ elety : chr [1:3459] "N" "CA" "C" "O" ...  
## ..$ alt : chr [1:3459] NA NA NA NA ...  
## ..$ resid : chr [1:3459] "MET" "MET" "MET" "MET" ...  
## ..$ chain : chr [1:3459] "A" "A" "A" "A" ...  
## ..$ resno : int [1:3459] 1 1 1 1 1 1 1 1 2 2 ...  
## ..$ insert: chr [1:3459] NA NA NA NA ...  
## ..$ x : num [1:3459] -10.93 -9.9 -9.17 -9.8 -10.59 ...  
## ..$ y : num [1:3459] -24.9 -24.4 -23.3 -22.3 -24 ...  
## ..$ z : num [1:3459] -9.52 -10.48 -9.81 -9.35 -11.77 ...  
## ..$ o : num [1:3459] 1 1 1 1 1 1 1 1 1 1 ...  
## ..$ b : num [1:3459] 41.5 29 27.9 26.4 34.2 ...  
## ..$ segid : chr [1:3459] NA NA NA NA ...  
## ..$ elesy : chr [1:3459] "N" "C" "C" "O" ...  
## ..$ charge: chr [1:3459] NA NA NA NA ...  
## $ xyz : 'xyz' num [1, 1:10377] -10.93 -24.89 -9.52 -9.9 -24.42 ...  
## $ seqres: Named chr [1:428] "MET" "ARG" "ILE" "ILE" ...  
## ..- attr(\*, "names")= chr [1:428] "A" "A" "A" "A" ...  
## $ helix :List of 4  
## ..$ start: Named num [1:19] 13 31 44 61 75 90 113 161 202 13 ...  
## .. ..- attr(\*, "names")= chr [1:19] "" "" "" "" ...  
## ..$ end : Named num [1:19] 24 40 54 73 77 98 121 187 213 24 ...  
## .. ..- attr(\*, "names")= chr [1:19] "" "" "" "" ...  
## ..$ chain: chr [1:19] "A" "A" "A" "A" ...  
## ..$ type : chr [1:19] "5" "1" "1" "1" ...  
## $ sheet :List of 4  
## ..$ start: Named num [1:14] 192 105 2 81 27 123 131 192 105 2 ...  
## .. ..- attr(\*, "names")= chr [1:14] "" "" "" "" ...  
## ..$ end : Named num [1:14] 197 110 7 84 29 126 134 197 110 7 ...  
## .. ..- attr(\*, "names")= chr [1:14] "" "" "" "" ...  
## ..$ chain: chr [1:14] "A" "A" "A" "A" ...  
## ..$ sense: chr [1:14] "0" "1" "1" "1" ...  
## $ calpha: logi [1:3459] FALSE TRUE FALSE FALSE FALSE FALSE ...  
## $ remark:List of 1  
## ..$ biomat:List of 4  
## .. ..$ num : int 1  
## .. ..$ chain :List of 1  
## .. .. ..$ : chr [1:2] "A" "B"  
## .. ..$ mat :List of 1  
## .. .. ..$ :List of 1  
## .. .. .. ..$ A B: num [1:3, 1:4] 1 0 0 0 1 0 0 0 1 0 ...  
## .. ..$ method: chr "AUTHOR"  
## $ call : language read.pdb(file = "4AKE")  
## - attr(\*, "class")= chr [1:2] "pdb" "sse"

s1$seqres

## A A A A A A A A A A A A A   
## "MET" "ARG" "ILE" "ILE" "LEU" "LEU" "GLY" "ALA" "PRO" "GLY" "ALA" "GLY" "LYS"   
## A A A A A A A A A A A A A   
## "GLY" "THR" "GLN" "ALA" "GLN" "PHE" "ILE" "MET" "GLU" "LYS" "TYR" "GLY" "ILE"   
## A A A A A A A A A A A A A   
## "PRO" "GLN" "ILE" "SER" "THR" "GLY" "ASP" "MET" "LEU" "ARG" "ALA" "ALA" "VAL"   
## A A A A A A A A A A A A A   
## "LYS" "SER" "GLY" "SER" "GLU" "LEU" "GLY" "LYS" "GLN" "ALA" "LYS" "ASP" "ILE"   
## A A A A A A A A A A A A A   
## "MET" "ASP" "ALA" "GLY" "LYS" "LEU" "VAL" "THR" "ASP" "GLU" "LEU" "VAL" "ILE"   
## A A A A A A A A A A A A A   
## "ALA" "LEU" "VAL" "LYS" "GLU" "ARG" "ILE" "ALA" "GLN" "GLU" "ASP" "CYS" "ARG"   
## A A A A A A A A A A A A A   
## "ASN" "GLY" "PHE" "LEU" "LEU" "ASP" "GLY" "PHE" "PRO" "ARG" "THR" "ILE" "PRO"   
## A A A A A A A A A A A A A   
## "GLN" "ALA" "ASP" "ALA" "MET" "LYS" "GLU" "ALA" "GLY" "ILE" "ASN" "VAL" "ASP"   
## A A A A A A A A A A A A A   
## "TYR" "VAL" "LEU" "GLU" "PHE" "ASP" "VAL" "PRO" "ASP" "GLU" "LEU" "ILE" "VAL"   
## A A A A A A A A A A A A A   
## "ASP" "ARG" "ILE" "VAL" "GLY" "ARG" "ARG" "VAL" "HIS" "ALA" "PRO" "SER" "GLY"   
## A A A A A A A A A A A A A   
## "ARG" "VAL" "TYR" "HIS" "VAL" "LYS" "PHE" "ASN" "PRO" "PRO" "LYS" "VAL" "GLU"   
## A A A A A A A A A A A A A   
## "GLY" "LYS" "ASP" "ASP" "VAL" "THR" "GLY" "GLU" "GLU" "LEU" "THR" "THR" "ARG"   
## A A A A A A A A A A A A A   
## "LYS" "ASP" "ASP" "GLN" "GLU" "GLU" "THR" "VAL" "ARG" "LYS" "ARG" "LEU" "VAL"   
## A A A A A A A A A A A A A   
## "GLU" "TYR" "HIS" "GLN" "MET" "THR" "ALA" "PRO" "LEU" "ILE" "GLY" "TYR" "TYR"   
## A A A A A A A A A A A A A   
## "SER" "LYS" "GLU" "ALA" "GLU" "ALA" "GLY" "ASN" "THR" "LYS" "TYR" "ALA" "LYS"   
## A A A A A A A A A A A A A   
## "VAL" "ASP" "GLY" "THR" "LYS" "PRO" "VAL" "ALA" "GLU" "VAL" "ARG" "ALA" "ASP"   
## A A A A A A B B B B B B B   
## "LEU" "GLU" "LYS" "ILE" "LEU" "GLY" "MET" "ARG" "ILE" "ILE" "LEU" "LEU" "GLY"   
## B B B B B B B B B B B B B   
## "ALA" "PRO" "GLY" "ALA" "GLY" "LYS" "GLY" "THR" "GLN" "ALA" "GLN" "PHE" "ILE"   
## B B B B B B B B B B B B B   
## "MET" "GLU" "LYS" "TYR" "GLY" "ILE" "PRO" "GLN" "ILE" "SER" "THR" "GLY" "ASP"   
## B B B B B B B B B B B B B   
## "MET" "LEU" "ARG" "ALA" "ALA" "VAL" "LYS" "SER" "GLY" "SER" "GLU" "LEU" "GLY"   
## B B B B B B B B B B B B B   
## "LYS" "GLN" "ALA" "LYS" "ASP" "ILE" "MET" "ASP" "ALA" "GLY" "LYS" "LEU" "VAL"   
## B B B B B B B B B B B B B   
## "THR" "ASP" "GLU" "LEU" "VAL" "ILE" "ALA" "LEU" "VAL" "LYS" "GLU" "ARG" "ILE"   
## B B B B B B B B B B B B B   
## "ALA" "GLN" "GLU" "ASP" "CYS" "ARG" "ASN" "GLY" "PHE" "LEU" "LEU" "ASP" "GLY"   
## B B B B B B B B B B B B B   
## "PHE" "PRO" "ARG" "THR" "ILE" "PRO" "GLN" "ALA" "ASP" "ALA" "MET" "LYS" "GLU"   
## B B B B B B B B B B B B B   
## "ALA" "GLY" "ILE" "ASN" "VAL" "ASP" "TYR" "VAL" "LEU" "GLU" "PHE" "ASP" "VAL"   
## B B B B B B B B B B B B B   
## "PRO" "ASP" "GLU" "LEU" "ILE" "VAL" "ASP" "ARG" "ILE" "VAL" "GLY" "ARG" "ARG"   
## B B B B B B B B B B B B B   
## "VAL" "HIS" "ALA" "PRO" "SER" "GLY" "ARG" "VAL" "TYR" "HIS" "VAL" "LYS" "PHE"   
## B B B B B B B B B B B B B   
## "ASN" "PRO" "PRO" "LYS" "VAL" "GLU" "GLY" "LYS" "ASP" "ASP" "VAL" "THR" "GLY"   
## B B B B B B B B B B B B B   
## "GLU" "GLU" "LEU" "THR" "THR" "ARG" "LYS" "ASP" "ASP" "GLN" "GLU" "GLU" "THR"   
## B B B B B B B B B B B B B   
## "VAL" "ARG" "LYS" "ARG" "LEU" "VAL" "GLU" "TYR" "HIS" "GLN" "MET" "THR" "ALA"   
## B B B B B B B B B B B B B   
## "PRO" "LEU" "ILE" "GLY" "TYR" "TYR" "SER" "LYS" "GLU" "ALA" "GLU" "ALA" "GLY"   
## B B B B B B B B B B B B B   
## "ASN" "THR" "LYS" "TYR" "ALA" "LYS" "VAL" "ASP" "GLY" "THR" "LYS" "PRO" "VAL"   
## B B B B B B B B B B B B   
## "ALA" "GLU" "VAL" "ARG" "ALA" "ASP" "LEU" "GLU" "LYS" "ILE" "LEU" "GLY"

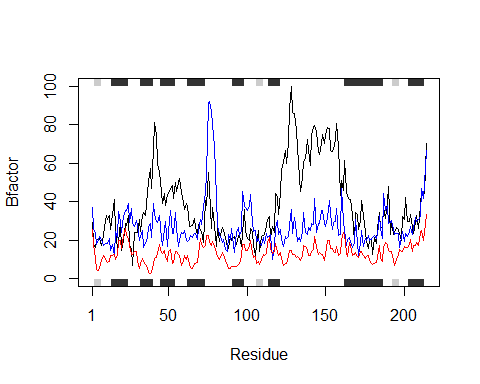
aa321(s1$seqres)

## [1] "M" "R" "I" "I" "L" "L" "G" "A" "P" "G" "A" "G" "K" "G" "T" "Q" "A" "Q"  
## [19] "F" "I" "M" "E" "K" "Y" "G" "I" "P" "Q" "I" "S" "T" "G" "D" "M" "L" "R"  
## [37] "A" "A" "V" "K" "S" "G" "S" "E" "L" "G" "K" "Q" "A" "K" "D" "I" "M" "D"  
## [55] "A" "G" "K" "L" "V" "T" "D" "E" "L" "V" "I" "A" "L" "V" "K" "E" "R" "I"  
## [73] "A" "Q" "E" "D" "C" "R" "N" "G" "F" "L" "L" "D" "G" "F" "P" "R" "T" "I"  
## [91] "P" "Q" "A" "D" "A" "M" "K" "E" "A" "G" "I" "N" "V" "D" "Y" "V" "L" "E"  
## [109] "F" "D" "V" "P" "D" "E" "L" "I" "V" "D" "R" "I" "V" "G" "R" "R" "V" "H"  
## [127] "A" "P" "S" "G" "R" "V" "Y" "H" "V" "K" "F" "N" "P" "P" "K" "V" "E" "G"  
## [145] "K" "D" "D" "V" "T" "G" "E" "E" "L" "T" "T" "R" "K" "D" "D" "Q" "E" "E"  
## [163] "T" "V" "R" "K" "R" "L" "V" "E" "Y" "H" "Q" "M" "T" "A" "P" "L" "I" "G"  
## [181] "Y" "Y" "S" "K" "E" "A" "E" "A" "G" "N" "T" "K" "Y" "A" "K" "V" "D" "G"  
## [199] "T" "K" "P" "V" "A" "E" "V" "R" "A" "D" "L" "E" "K" "I" "L" "G" "M" "R"  
## [217] "I" "I" "L" "L" "G" "A" "P" "G" "A" "G" "K" "G" "T" "Q" "A" "Q" "F" "I"  
## [235] "M" "E" "K" "Y" "G" "I" "P" "Q" "I" "S" "T" "G" "D" "M" "L" "R" "A" "A"  
## [253] "V" "K" "S" "G" "S" "E" "L" "G" "K" "Q" "A" "K" "D" "I" "M" "D" "A" "G"  
## [271] "K" "L" "V" "T" "D" "E" "L" "V" "I" "A" "L" "V" "K" "E" "R" "I" "A" "Q"  
## [289] "E" "D" "C" "R" "N" "G" "F" "L" "L" "D" "G" "F" "P" "R" "T" "I" "P" "Q"  
## [307] "A" "D" "A" "M" "K" "E" "A" "G" "I" "N" "V" "D" "Y" "V" "L" "E" "F" "D"  
## [325] "V" "P" "D" "E" "L" "I" "V" "D" "R" "I" "V" "G" "R" "R" "V" "H" "A" "P"  
## [343] "S" "G" "R" "V" "Y" "H" "V" "K" "F" "N" "P" "P" "K" "V" "E" "G" "K" "D"  
## [361] "D" "V" "T" "G" "E" "E" "L" "T" "T" "R" "K" "D" "D" "Q" "E" "E" "T" "V"  
## [379] "R" "K" "R" "L" "V" "E" "Y" "H" "Q" "M" "T" "A" "P" "L" "I" "G" "Y" "Y"  
## [397] "S" "K" "E" "A" "E" "A" "G" "N" "T" "K" "Y" "A" "K" "V" "D" "G" "T" "K"  
## [415] "P" "V" "A" "E" "V" "R" "A" "D" "L" "E" "K" "I" "L" "G"

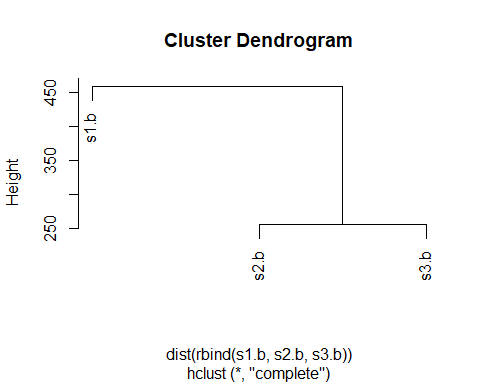
s1$atom

## type eleno elety alt resid chain resno insert x y z  
## 1 ATOM 1 N <NA> MET A 1 <NA> -10.928 -24.892 -9.518  
## 2 ATOM 2 CA <NA> MET A 1 <NA> -9.901 -24.422 -10.479  
## 3 ATOM 3 C <NA> MET A 1 <NA> -9.168 -23.266 -9.813  
## 4 ATOM 4 O <NA> MET A 1 <NA> -9.802 -22.323 -9.346  
## 5 ATOM 5 CB <NA> MET A 1 <NA> -10.585 -23.970 -11.774  
## 6 ATOM 6 CG <NA> MET A 1 <NA> -9.650 -23.497 -12.856  
## 7 ATOM 7 SD <NA> MET A 1 <NA> -8.384 -24.690 -13.251  
## 8 ATOM 8 CE <NA> MET A 1 <NA> -9.002 -25.277 -14.812  
## 9 ATOM 9 N <NA> ARG A 2 <NA> -7.851 -23.394 -9.673  
## 10 ATOM 10 CA <NA> ARG A 2 <NA> -7.028 -22.352 -9.051  
## 11 ATOM 11 C <NA> ARG A 2 <NA> -6.001 -21.906 -10.072  
## 12 ATOM 12 O <NA> ARG A 2 <NA> -5.150 -22.680 -10.492  
## 13 ATOM 13 CB <NA> ARG A 2 <NA> -6.337 -22.868 -7.801  
## 14 ATOM 14 CG <NA> ARG A 2 <NA> -7.222 -22.919 -6.621  
## 15 ATOM 15 CD <NA> ARG A 2 <NA> -6.632 -23.799 -5.576  
## 16 ATOM 16 NE <NA> ARG A 2 <NA> -7.440 -23.763 -4.372  
## 17 ATOM 17 CZ <NA> ARG A 2 <NA> -6.965 -23.881 -3.138  
## 18 ATOM 18 NH1 <NA> ARG A 2 <NA> -5.664 -24.050 -2.932  
## 19 ATOM 19 NH2 <NA> ARG A 2 <NA> -7.806 -23.818 -2.112  
## 20 ATOM 20 N <NA> ILE A 3 <NA> -6.082 -20.641 -10.448  
## 21 ATOM 21 CA <NA> ILE A 3 <NA> -5.227 -20.106 -11.463  
## 22 ATOM 22 C <NA> ILE A 3 <NA> -4.540 -18.831 -10.985  
## 23 ATOM 23 O <NA> ILE A 3 <NA> -5.118 -18.060 -10.228  
## 24 ATOM 24 CB <NA> ILE A 3 <NA> -6.098 -19.813 -12.702  
## 25 ATOM 25 CG1 <NA> ILE A 3 <NA> -6.670 -21.108 -13.263  
## 26 ATOM 26 CG2 <NA> ILE A 3 <NA> -5.337 -19.077 -13.744  
## 27 ATOM 27 CD1 <NA> ILE A 3 <NA> -7.875 -20.870 -14.122  
## 28 ATOM 28 N <NA> ILE A 4 <NA> -3.263 -18.691 -11.331  
## 29 ATOM 29 CA <NA> ILE A 4 <NA> -2.477 -17.496 -11.033  
## 30 ATOM 30 C <NA> ILE A 4 <NA> -2.299 -16.916 -12.455  
## 31 ATOM 31 O <NA> ILE A 4 <NA> -1.920 -17.651 -13.376  
## 32 ATOM 32 CB <NA> ILE A 4 <NA> -1.088 -17.867 -10.428  
## 33 ATOM 33 CG1 <NA> ILE A 4 <NA> -1.254 -18.305 -8.975  
## 34 ATOM 34 CG2 <NA> ILE A 4 <NA> -0.134 -16.690 -10.511  
## 35 ATOM 35 CD1 <NA> ILE A 4 <NA> -0.001 -18.800 -8.363  
## 36 ATOM 36 N <NA> LEU A 5 <NA> -2.663 -15.647 -12.649  
## 37 ATOM 37 CA <NA> LEU A 5 <NA> -2.565 -14.983 -13.957  
## 38 ATOM 38 C <NA> LEU A 5 <NA> -1.444 -13.957 -13.914  
## 39 ATOM 39 O <NA> LEU A 5 <NA> -1.535 -12.986 -13.177  
## 40 ATOM 40 CB <NA> LEU A 5 <NA> -3.905 -14.287 -14.286  
## 41 ATOM 41 CG <NA> LEU A 5 <NA> -4.199 -13.784 -15.709  
## 42 ATOM 42 CD1 <NA> LEU A 5 <NA> -4.065 -14.897 -16.723  
## 43 ATOM 43 CD2 <NA> LEU A 5 <NA> -5.602 -13.212 -15.783  
## 44 ATOM 44 N <NA> LEU A 6 <NA> -0.381 -14.186 -14.680  
## 45 ATOM 45 CA <NA> LEU A 6 <NA> 0.768 -13.265 -14.734  
## 46 ATOM 46 C <NA> LEU A 6 <NA> 0.775 -12.442 -16.033  
## 47 ATOM 47 O <NA> LEU A 6 <NA> 0.313 -12.896 -17.077  
## 48 ATOM 48 CB <NA> LEU A 6 <NA> 2.097 -14.034 -14.657  
## 49 ATOM 49 CG <NA> LEU A 6 <NA> 2.441 -14.999 -13.526  
## 50 ATOM 50 CD1 <NA> LEU A 6 <NA> 3.800 -15.554 -13.804  
## 51 ATOM 51 CD2 <NA> LEU A 6 <NA> 2.436 -14.323 -12.202  
## 52 ATOM 52 N <NA> GLY A 7 <NA> 1.347 -11.252 -15.980  
## 53 ATOM 53 CA <NA> GLY A 7 <NA> 1.394 -10.431 -17.162  
## 54 ATOM 54 C <NA> GLY A 7 <NA> 1.994 -9.074 -16.883  
## 55 ATOM 55 O <NA> GLY A 7 <NA> 1.782 -8.467 -15.829  
## 56 ATOM 56 N <NA> ALA A 8 <NA> 2.748 -8.581 -17.852  
## 57 ATOM 57 CA <NA> ALA A 8 <NA> 3.395 -7.286 -17.735  
## 58 ATOM 58 C <NA> ALA A 8 <NA> 2.367 -6.186 -17.693  
## 59 ATOM 59 O <NA> ALA A 8 <NA> 1.232 -6.380 -18.111  
## 60 ATOM 60 CB <NA> ALA A 8 <NA> 4.341 -7.053 -18.932  
## 61 ATOM 61 N <NA> PRO A 9 <NA> 2.703 -5.066 -17.048  
## 62 ATOM 62 CA <NA> PRO A 9 <NA> 1.751 -3.951 -17.001  
## 63 ATOM 63 C <NA> PRO A 9 <NA> 1.553 -3.408 -18.438  
## 64 ATOM 64 O <NA> PRO A 9 <NA> 2.522 -3.054 -19.124  
## 65 ATOM 65 CB <NA> PRO A 9 <NA> 2.471 -2.924 -16.105  
## 66 ATOM 66 CG <NA> PRO A 9 <NA> 3.927 -3.344 -16.139  
## 67 ATOM 67 CD <NA> PRO A 9 <NA> 3.824 -4.836 -16.122  
## 68 ATOM 68 N <NA> GLY A 10 <NA> 0.310 -3.411 -18.905  
## 69 ATOM 69 CA <NA> GLY A 10 <NA> 0.015 -2.928 -20.242  
## 70 ATOM 70 C <NA> GLY A 10 <NA> -0.312 -4.025 -21.253  
## 71 ATOM 71 O <NA> GLY A 10 <NA> -0.853 -3.739 -22.326  
## 72 ATOM 72 N <NA> ALA A 11 <NA> 0.000 -5.277 -20.915  
## 73 ATOM 73 CA <NA> ALA A 11 <NA> -0.245 -6.408 -21.794  
## 74 ATOM 74 C <NA> ALA A 11 <NA> -1.725 -6.790 -21.936  
## 75 ATOM 75 O <NA> ALA A 11 <NA> -2.084 -7.520 -22.854  
## 76 ATOM 76 CB <NA> ALA A 11 <NA> 0.572 -7.611 -21.333  
## 77 ATOM 77 N <NA> GLY A 12 <NA> -2.573 -6.323 -21.019  
## 78 ATOM 78 CA <NA> GLY A 12 <NA> -3.997 -6.640 -21.064  
## 79 ATOM 79 C <NA> GLY A 12 <NA> -4.390 -8.078 -20.715  
## 80 ATOM 80 O <NA> GLY A 12 <NA> -5.149 -8.694 -21.467  
## 81 ATOM 81 N <NA> LYS A 13 <NA> -3.911 -8.616 -19.584  
## 82 ATOM 82 CA <NA> LYS A 13 <NA> -4.260 -9.988 -19.188  
## 83 ATOM 83 C <NA> LYS A 13 <NA> -5.680 -10.006 -18.658  
## 84 ATOM 84 O <NA> LYS A 13 <NA> -6.353 -11.031 -18.675  
## 85 ATOM 85 CB <NA> LYS A 13 <NA> -3.286 -10.535 -18.139  
## 86 ATOM 86 CG <NA> LYS A 13 <NA> -3.122 -9.642 -16.939  
## 87 ATOM 87 CD <NA> LYS A 13 <NA> -2.311 -10.303 -15.863  
## 88 ATOM 88 CE <NA> LYS A 13 <NA> -2.551 -9.626 -14.520  
## 89 ATOM 89 NZ <NA> LYS A 13 <NA> -1.805 -8.367 -14.274  
## 90 ATOM 90 N <NA> GLY A 14 <NA> -6.132 -8.842 -18.217  
## 91 ATOM 91 CA <NA> GLY A 14 <NA> -7.477 -8.701 -17.702  
## 92 ATOM 92 C <NA> GLY A 14 <NA> -8.531 -9.048 -18.735  
## 93 ATOM 93 O <NA> GLY A 14 <NA> -9.626 -9.484 -18.386  
## 94 ATOM 94 N <NA> THR A 15 <NA> -8.180 -8.934 -20.010  
## 95 ATOM 95 CA <NA> THR A 15 <NA> -9.115 -9.225 -21.105  
## 96 ATOM 96 C <NA> THR A 15 <NA> -9.729 -10.637 -21.047  
## 97 ATOM 97 O <NA> THR A 15 <NA> -10.866 -10.859 -21.471  
## 98 ATOM 98 CB <NA> THR A 15 <NA> -8.445 -9.008 -22.522  
## 99 ATOM 99 OG1 <NA> THR A 15 <NA> -7.462 -10.028 -22.777  
## 100 ATOM 100 CG2 <NA> THR A 15 <NA> -7.795 -7.613 -22.614  
## 101 ATOM 101 N <NA> GLN A 16 <NA> -9.003 -11.575 -20.468  
## 102 ATOM 102 CA <NA> GLN A 16 <NA> -9.497 -12.931 -20.423  
## 103 ATOM 103 C <NA> GLN A 16 <NA> -10.070 -13.344 -19.064  
## 104 ATOM 104 O <NA> GLN A 16 <NA> -10.578 -14.443 -18.909  
## 105 ATOM 105 CB <NA> GLN A 16 <NA> -8.375 -13.859 -20.883  
## 106 ATOM 106 CG <NA> GLN A 16 <NA> -8.764 -14.832 -22.010  
## 107 ATOM 107 CD <NA> GLN A 16 <NA> -9.211 -14.179 -23.318  
## 108 ATOM 108 OE1 <NA> GLN A 16 <NA> -8.426 -13.538 -24.023  
## 109 ATOM 109 NE2 <NA> GLN A 16 <NA> -10.471 -14.401 -23.676  
## 110 ATOM 110 N <NA> ALA A 17 <NA> -10.089 -12.417 -18.121  
## 111 ATOM 111 CA <NA> ALA A 17 <NA> -10.578 -12.687 -16.783  
## 112 ATOM 112 C <NA> ALA A 17 <NA> -12.046 -13.047 -16.702  
## 113 ATOM 113 O <NA> ALA A 17 <NA> -12.398 -14.055 -16.087  
## 114 ATOM 114 CB <NA> ALA A 17 <NA> -10.276 -11.528 -15.885  
## 115 ATOM 115 N <NA> GLN A 18 <NA> -12.919 -12.231 -17.286  
## 116 ATOM 116 CA <NA> GLN A 18 <NA> -14.357 -12.543 -17.256  
## 117 ATOM 117 C <NA> GLN A 18 <NA> -14.621 -13.930 -17.792  
## 118 ATOM 118 O <NA> GLN A 18 <NA> -15.469 -14.647 -17.276  
## 119 ATOM 119 CB <NA> GLN A 18 <NA> -15.158 -11.560 -18.094  
## 120 ATOM 120 CG <NA> GLN A 18 <NA> -15.836 -10.454 -17.315  
## 121 ATOM 121 CD <NA> GLN A 18 <NA> -16.874 -9.740 -18.151  
## 122 ATOM 122 OE1 <NA> GLN A 18 <NA> -17.676 -10.377 -18.855  
## 123 ATOM 123 NE2 <NA> GLN A 18 <NA> -16.866 -8.410 -18.090  
## 124 ATOM 124 N <NA> PHE A 19 <NA> -13.902 -14.307 -18.842  
## 125 ATOM 125 CA <NA> PHE A 19 <NA> -14.086 -15.630 -19.436  
## 126 ATOM 126 C <NA> PHE A 19 <NA> -13.799 -16.726 -18.404  
## 127 ATOM 127 O <NA> PHE A 19 <NA> -14.609 -17.626 -18.168  
## 128 ATOM 128 CB <NA> PHE A 19 <NA> -13.189 -15.776 -20.691  
## 129 ATOM 129 CG <NA> PHE A 19 <NA> -12.957 -17.207 -21.123  
## 130 ATOM 130 CD1 <NA> PHE A 19 <NA> -14.010 -18.000 -21.575  
## 131 ATOM 131 CD2 <NA> PHE A 19 <NA> -11.689 -17.782 -21.014  
## 132 ATOM 132 CE1 <NA> PHE A 19 <NA> -13.804 -19.340 -21.900  
## 133 ATOM 133 CE2 <NA> PHE A 19 <NA> -11.471 -19.120 -21.337  
## 134 ATOM 134 CZ <NA> PHE A 19 <NA> -12.527 -19.899 -21.778  
## 135 ATOM 135 N <NA> ILE A 20 <NA> -12.648 -16.616 -17.767  
## 136 ATOM 136 CA <NA> ILE A 20 <NA> -12.235 -17.560 -16.776  
## 137 ATOM 137 C <NA> ILE A 20 <NA> -13.256 -17.654 -15.644  
## 138 ATOM 138 O <NA> ILE A 20 <NA> -13.676 -18.743 -15.305  
## 139 ATOM 139 CB <NA> ILE A 20 <NA> -10.849 -17.187 -16.276  
## 140 ATOM 140 CG1 <NA> ILE A 20 <NA> -9.866 -17.333 -17.431  
## 141 ATOM 141 CG2 <NA> ILE A 20 <NA> -10.417 -18.105 -15.144  
## 142 ATOM 142 CD1 <NA> ILE A 20 <NA> -8.545 -16.770 -17.128  
## 143 ATOM 143 N <NA> MET A 21 <NA> -13.705 -16.535 -15.090  
## 144 ATOM 144 CA <NA> MET A 21 <NA> -14.712 -16.590 -14.022  
## 145 ATOM 145 C <NA> MET A 21 <NA> -15.991 -17.276 -14.527  
## 146 ATOM 146 O <NA> MET A 21 <NA> -16.523 -18.220 -13.909  
## 147 ATOM 147 CB <NA> MET A 21 <NA> -15.056 -15.189 -13.545  
## 148 ATOM 148 CG <NA> MET A 21 <NA> -13.957 -14.482 -12.818  
## 149 ATOM 149 SD <NA> MET A 21 <NA> -14.247 -12.668 -12.731  
## 150 ATOM 150 CE <NA> MET A 21 <NA> -15.099 -12.499 -11.289  
## 151 ATOM 151 N <NA> GLU A 22 <NA> -16.432 -16.846 -15.699  
## 152 ATOM 152 CA <NA> GLU A 22 <NA> -17.629 -17.379 -16.311  
## 153 ATOM 153 C <NA> GLU A 22 <NA> -17.538 -18.848 -16.683  
## 154 ATOM 154 O <NA> GLU A 22 <NA> -18.543 -19.553 -16.679  
## 155 ATOM 155 CB <NA> GLU A 22 <NA> -17.984 -16.553 -17.535  
## 156 ATOM 156 CG <NA> GLU A 22 <NA> -19.271 -16.996 -18.223  
## 157 ATOM 157 CD <NA> GLU A 22 <NA> -20.171 -15.833 -18.616  
## 158 ATOM 158 OE1 <NA> GLU A 22 <NA> -19.661 -14.689 -18.762  
## 159 ATOM 159 OE2 <NA> GLU A 22 <NA> -21.395 -16.069 -18.773  
## 160 ATOM 160 N <NA> LYS A 23 <NA> -16.347 -19.333 -16.988  
## 161 ATOM 161 CA <NA> LYS A 23 <NA> -16.228 -20.729 -17.365  
## 162 ATOM 162 C <NA> LYS A 23 <NA> -16.122 -21.678 -16.154  
## 163 ATOM 163 O <NA> LYS A 23 <NA> -16.657 -22.792 -16.164  
## 164 ATOM 164 CB <NA> LYS A 23 <NA> -15.026 -20.897 -18.290  
## 165 ATOM 165 CG <NA> LYS A 23 <NA> -15.163 -22.045 -19.276  
## 166 ATOM 166 CD <NA> LYS A 23 <NA> -16.377 -21.832 -20.188  
## 167 ATOM 167 CE <NA> LYS A 23 <NA> -16.556 -22.984 -21.169  
## 168 ATOM 168 NZ <NA> LYS A 23 <NA> -16.822 -24.278 -20.472  
## 169 ATOM 169 N <NA> TYR A 24 <NA> -15.475 -21.213 -15.089  
## 170 ATOM 170 CA <NA> TYR A 24 <NA> -15.265 -22.028 -13.897  
## 171 ATOM 171 C <NA> TYR A 24 <NA> -16.073 -21.622 -12.656  
## 172 ATOM 172 O <NA> TYR A 24 <NA> -16.139 -22.371 -11.694  
## 173 ATOM 173 CB <NA> TYR A 24 <NA> -13.750 -22.093 -13.590  
## 174 ATOM 174 CG <NA> TYR A 24 <NA> -12.969 -22.520 -14.814  
## 175 ATOM 175 CD1 <NA> TYR A 24 <NA> -12.867 -23.870 -15.169  
## 176 ATOM 176 CD2 <NA> TYR A 24 <NA> -12.507 -21.570 -15.724  
## 177 ATOM 177 CE1 <NA> TYR A 24 <NA> -12.343 -24.257 -16.419  
## 178 ATOM 178 CE2 <NA> TYR A 24 <NA> -11.990 -21.940 -16.970  
## 179 ATOM 179 CZ <NA> TYR A 24 <NA> -11.918 -23.280 -17.321  
## 180 ATOM 180 OH <NA> TYR A 24 <NA> -11.500 -23.611 -18.598  
## 181 ATOM 181 N <NA> GLY A 25 <NA> -16.699 -20.456 -12.680  
## 182 ATOM 182 CA <NA> GLY A 25 <NA> -17.460 -20.048 -11.528  
## 183 ATOM 183 C <NA> GLY A 25 <NA> -16.562 -19.793 -10.351  
## 184 ATOM 184 O <NA> GLY A 25 <NA> -16.817 -20.284 -9.254  
## 185 ATOM 185 N <NA> ILE A 26 <NA> -15.548 -18.957 -10.573  
## 186 ATOM 186 CA <NA> ILE A 26 <NA> -14.555 -18.595 -9.561  
## 187 ATOM 187 C <NA> ILE A 26 <NA> -14.380 -17.090 -9.634  
## 188 ATOM 188 O <NA> ILE A 26 <NA> -14.632 -16.480 -10.665  
## 189 ATOM 189 CB <NA> ILE A 26 <NA> -13.164 -19.303 -9.802  
## 190 ATOM 190 CG1 <NA> ILE A 26 <NA> -12.495 -18.788 -11.065  
## 191 ATOM 191 CG2 <NA> ILE A 26 <NA> -13.329 -20.795 -9.973  
## 192 ATOM 192 CD1 <NA> ILE A 26 <NA> -11.387 -19.642 -11.530  
## 193 ATOM 193 N <NA> PRO A 27 <NA> -14.005 -16.463 -8.519  
## 194 ATOM 194 CA <NA> PRO A 27 <NA> -13.805 -15.020 -8.472  
## 195 ATOM 195 C <NA> PRO A 27 <NA> -12.377 -14.587 -8.719  
## 196 ATOM 196 O <NA> PRO A 27 <NA> -11.440 -15.361 -8.564  
## 197 ATOM 197 CB <NA> PRO A 27 <NA> -14.203 -14.694 -7.044  
## 198 ATOM 198 CG <NA> PRO A 27 <NA> -13.650 -15.859 -6.292  
## 199 ATOM 199 CD <NA> PRO A 27 <NA> -14.069 -17.029 -7.158  
## 200 ATOM 200 N <NA> GLN A 28 <NA> -12.216 -13.307 -9.015  
## 201 ATOM 201 CA <NA> GLN A 28 <NA> -10.906 -12.712 -9.244  
## 202 ATOM 202 C <NA> GLN A 28 <NA> -10.476 -12.047 -7.951  
## 203 ATOM 203 O <NA> GLN A 28 <NA> -11.169 -11.188 -7.415  
## 204 ATOM 204 CB <NA> GLN A 28 <NA> -10.968 -11.652 -10.340  
## 205 ATOM 205 CG <NA> GLN A 28 <NA> -9.661 -10.934 -10.562  
## 206 ATOM 206 CD <NA> GLN A 28 <NA> -9.785 -9.770 -11.526  
## 207 ATOM 207 OE1 <NA> GLN A 28 <NA> -10.646 -9.759 -12.405  
## 208 ATOM 208 NE2 <NA> GLN A 28 <NA> -8.915 -8.781 -11.367  
## 209 ATOM 209 N <NA> ILE A 29 <NA> -9.334 -12.464 -7.439  
## 210 ATOM 210 CA <NA> ILE A 29 <NA> -8.804 -11.920 -6.211  
## 211 ATOM 211 C <NA> ILE A 29 <NA> -7.555 -11.176 -6.615  
## 212 ATOM 212 O <NA> ILE A 29 <NA> -6.773 -11.667 -7.417  
## 213 ATOM 213 CB <NA> ILE A 29 <NA> -8.363 -13.054 -5.255  
## 214 ATOM 214 CG1 <NA> ILE A 29 <NA> -9.536 -13.970 -4.895  
## 215 ATOM 215 CG2 <NA> ILE A 29 <NA> -7.696 -12.466 -4.013  
## 216 ATOM 216 CD1 <NA> ILE A 29 <NA> -9.074 -15.271 -4.274  
## 217 ATOM 217 N <NA> SER A 30 <NA> -7.388 -9.976 -6.103  
## 218 ATOM 218 CA <NA> SER A 30 <NA> -6.192 -9.217 -6.380  
## 219 ATOM 219 C <NA> SER A 30 <NA> -5.840 -8.669 -4.993  
## 220 ATOM 220 O <NA> SER A 30 <NA> -6.728 -8.414 -4.181  
## 221 ATOM 221 CB <NA> SER A 30 <NA> -6.471 -8.124 -7.404  
## 222 ATOM 222 OG <NA> SER A 30 <NA> -6.760 -6.891 -6.774  
## 223 ATOM 223 N <NA> THR A 31 <NA> -4.555 -8.536 -4.691  
## 224 ATOM 224 CA <NA> THR A 31 <NA> -4.144 -8.071 -3.369  
## 225 ATOM 225 C <NA> THR A 31 <NA> -4.637 -6.676 -2.996  
## 226 ATOM 226 O <NA> THR A 31 <NA> -4.948 -6.412 -1.835  
## 227 ATOM 227 CB <NA> THR A 31 <NA> -2.593 -8.247 -3.148  
## 228 ATOM 228 OG1 <NA> THR A 31 <NA> -1.849 -7.434 -4.063  
## 229 ATOM 229 CG2 <NA> THR A 31 <NA> -2.210 -9.695 -3.398  
## 230 ATOM 230 N <NA> GLY A 32 <NA> -4.779 -5.802 -3.983  
## 231 ATOM 231 CA <NA> GLY A 32 <NA> -5.246 -4.466 -3.685  
## 232 ATOM 232 C <NA> GLY A 32 <NA> -6.683 -4.515 -3.226  
## 233 ATOM 233 O <NA> GLY A 32 <NA> -7.057 -3.825 -2.293  
## 234 ATOM 234 N <NA> ASP A 33 <NA> -7.482 -5.373 -3.848  
## 235 ATOM 235 CA <NA> ASP A 33 <NA> -8.898 -5.497 -3.509  
## 236 ATOM 236 C <NA> ASP A 33 <NA> -9.059 -6.134 -2.161  
## 237 ATOM 237 O <NA> ASP A 33 <NA> -9.866 -5.709 -1.347  
## 238 ATOM 238 CB <NA> ASP A 33 <NA> -9.636 -6.366 -4.537  
## 239 ATOM 239 CG <NA> ASP A 33 <NA> -9.907 -5.641 -5.870  
## 240 ATOM 240 OD1 <NA> ASP A 33 <NA> -9.956 -4.385 -5.901  
## 241 ATOM 241 OD2 <NA> ASP A 33 <NA> -10.093 -6.345 -6.897  
## 242 ATOM 242 N <NA> MET A 34 <NA> -8.293 -7.191 -1.959  
## 243 ATOM 243 CA <NA> MET A 34 <NA> -8.292 -7.982 -0.738  
## 244 ATOM 244 C <NA> MET A 34 <NA> -7.916 -7.163 0.471  
## 245 ATOM 245 O <NA> MET A 34 <NA> -8.541 -7.301 1.510  
## 246 ATOM 246 CB <NA> MET A 34 <NA> -7.297 -9.099 -0.907  
## 247 ATOM 247 CG <NA> MET A 34 <NA> -7.453 -10.222 0.027  
## 248 ATOM 248 SD <NA> MET A 34 <NA> -6.315 -11.395 -0.602  
## 249 ATOM 249 CE <NA> MET A 34 <NA> -4.810 -10.551 -0.080  
## 250 ATOM 250 N <NA> LEU A 35 <NA> -6.861 -6.358 0.341  
## 251 ATOM 251 CA <NA> LEU A 35 <NA> -6.401 -5.481 1.410  
## 252 ATOM 252 C <NA> LEU A 35 <NA> -7.534 -4.558 1.789  
## 253 ATOM 253 O <NA> LEU A 35 <NA> -7.998 -4.564 2.925  
## 254 ATOM 254 CB <NA> LEU A 35 <NA> -5.237 -4.629 0.933  
## 255 ATOM 255 CG <NA> LEU A 35 <NA> -3.833 -5.097 1.279  
## 256 ATOM 256 CD1 <NA> LEU A 35 <NA> -2.837 -4.144 0.655  
## 257 ATOM 257 CD2 <NA> LEU A 35 <NA> -3.660 -5.108 2.778  
## 258 ATOM 258 N <NA> ARG A 36 <NA> -7.993 -3.785 0.812  
## 259 ATOM 259 CA <NA> ARG A 36 <NA> -9.098 -2.856 0.993  
## 260 ATOM 260 C <NA> ARG A 36 <NA> -10.378 -3.506 1.573  
## 261 ATOM 261 O <NA> ARG A 36 <NA> -11.255 -2.819 2.072  
## 262 ATOM 262 CB <NA> ARG A 36 <NA> -9.389 -2.132 -0.335  
## 263 ATOM 263 CG <NA> ARG A 36 <NA> -8.223 -1.237 -0.798  
## 264 ATOM 264 CD <NA> ARG A 36 <NA> -8.593 -0.309 -1.969  
## 265 ATOM 265 NE <NA> ARG A 36 <NA> -8.576 -0.973 -3.275  
## 266 ATOM 266 CZ <NA> ARG A 36 <NA> -7.488 -1.132 -4.035  
## 267 ATOM 267 NH1 <NA> ARG A 36 <NA> -6.310 -0.669 -3.637  
## 268 ATOM 268 NH2 <NA> ARG A 36 <NA> -7.573 -1.752 -5.206  
## 269 ATOM 269 N <NA> ALA A 37 <NA> -10.457 -4.828 1.555  
## 270 ATOM 270 CA <NA> ALA A 37 <NA> -11.616 -5.549 2.081  
## 271 ATOM 271 C <NA> ALA A 37 <NA> -11.402 -6.114 3.499  
## 272 ATOM 272 O <NA> ALA A 37 <NA> -12.363 -6.482 4.188  
## 273 ATOM 273 CB <NA> ALA A 37 <NA> -11.990 -6.680 1.131  
## 274 ATOM 274 N <NA> ALA A 38 <NA> -10.144 -6.235 3.917  
## 275 ATOM 275 CA <NA> ALA A 38 <NA> -9.824 -6.758 5.244  
## 276 ATOM 276 C <NA> ALA A 38 <NA> -10.029 -5.651 6.272  
## 277 ATOM 277 O <NA> ALA A 38 <NA> -10.565 -5.876 7.363  
## 278 ATOM 278 CB <NA> ALA A 38 <NA> -8.382 -7.254 5.269  
## 279 ATOM 279 N <NA> VAL A 39 <NA> -9.582 -4.457 5.901  
## 280 ATOM 280 CA <NA> VAL A 39 <NA> -9.687 -3.275 6.731  
## 281 ATOM 281 C <NA> VAL A 39 <NA> -11.142 -3.086 7.134  
## 282 ATOM 282 O <NA> VAL A 39 <NA> -11.490 -3.199 8.307  
## 283 ATOM 283 CB <NA> VAL A 39 <NA> -9.160 -2.079 5.948  
## 284 ATOM 284 CG1 <NA> VAL A 39 <NA> -9.642 -0.774 6.535  
## 285 ATOM 285 CG2 <NA> VAL A 39 <NA> -7.659 -2.132 5.929  
## 286 ATOM 286 N <NA> LYS A 40 <NA> -11.982 -2.853 6.134  
## 287 ATOM 287 CA <NA> LYS A 40 <NA> -13.424 -2.667 6.301  
## 288 ATOM 288 C <NA> LYS A 40 <NA> -13.987 -3.665 7.299  
## 289 ATOM 289 O <NA> LYS A 40 <NA> -14.480 -3.278 8.357  
## 290 ATOM 290 CB <NA> LYS A 40 <NA> -14.113 -2.850 4.943  
## 291 ATOM 291 CG <NA> LYS A 40 <NA> -15.614 -3.110 4.970  
## 292 ATOM 292 CD <NA> LYS A 40 <NA> -16.107 -3.601 3.596  
## 293 ATOM 293 CE <NA> LYS A 40 <NA> -15.513 -4.978 3.218  
## 294 ATOM 294 NZ <NA> LYS A 40 <NA> -15.876 -5.463 1.844  
## 295 ATOM 295 N <NA> SER A 41 <NA> -13.931 -4.945 6.951  
## 296 ATOM 296 CA <NA> SER A 41 <NA> -14.424 -5.983 7.834  
## 297 ATOM 297 C <NA> SER A 41 <NA> -13.399 -6.205 8.925  
## 298 ATOM 298 O <NA> SER A 41 <NA> -12.667 -7.199 8.912  
## 299 ATOM 299 CB <NA> SER A 41 <NA> -14.679 -7.278 7.069  
## 300 ATOM 300 OG <NA> SER A 41 <NA> -15.944 -7.229 6.426  
## 301 ATOM 301 N <NA> GLY A 42 <NA> -13.357 -5.249 9.851  
## 302 ATOM 302 CA <NA> GLY A 42 <NA> -12.442 -5.274 10.976  
## 303 ATOM 303 C <NA> GLY A 42 <NA> -12.241 -6.624 11.622  
## 304 ATOM 304 O <NA> GLY A 42 <NA> -12.844 -6.951 12.639  
## 305 ATOM 305 N <NA> SER A 43 <NA> -11.419 -7.427 10.973  
## 306 ATOM 306 CA <NA> SER A 43 <NA> -11.066 -8.743 11.442  
## 307 ATOM 307 C <NA> SER A 43 <NA> -9.662 -8.524 12.000  
## 308 ATOM 308 O <NA> SER A 43 <NA> -9.067 -7.474 11.767  
## 309 ATOM 309 CB <NA> SER A 43 <NA> -11.052 -9.710 10.255  
## 310 ATOM 310 OG <NA> SER A 43 <NA> -10.553 -9.075 9.084  
## 311 ATOM 311 N <NA> GLU A 44 <NA> -9.130 -9.491 12.735  
## 312 ATOM 312 CA <NA> GLU A 44 <NA> -7.796 -9.348 13.305  
## 313 ATOM 313 C <NA> GLU A 44 <NA> -6.751 -8.878 12.279  
## 314 ATOM 314 O <NA> GLU A 44 <NA> -6.111 -7.846 12.473  
## 315 ATOM 315 CB <NA> GLU A 44 <NA> -7.367 -10.660 13.969  
## 316 ATOM 316 CG <NA> GLU A 44 <NA> -5.881 -10.754 14.342  
## 317 ATOM 317 CD <NA> GLU A 44 <NA> -5.455 -9.816 15.470  
## 318 ATOM 318 OE1 <NA> GLU A 44 <NA> -6.331 -9.186 16.117  
## 319 ATOM 319 OE2 <NA> GLU A 44 <NA> -4.227 -9.727 15.711  
## 320 ATOM 320 N <NA> LEU A 45 <NA> -6.608 -9.602 11.174  
## 321 ATOM 321 CA <NA> LEU A 45 <NA> -5.639 -9.232 10.148  
## 322 ATOM 322 C <NA> LEU A 45 <NA> -5.967 -7.886 9.489  
## 323 ATOM 323 O <NA> LEU A 45 <NA> -5.061 -7.085 9.213  
## 324 ATOM 324 CB <NA> LEU A 45 <NA> -5.546 -10.327 9.087  
## 325 ATOM 325 CG <NA> LEU A 45 <NA> -4.790 -11.604 9.463  
## 326 ATOM 326 CD1 <NA> LEU A 45 <NA> -3.305 -11.337 9.507  
## 327 ATOM 327 CD2 <NA> LEU A 45 <NA> -5.269 -12.129 10.809  
## 328 ATOM 328 N <NA> GLY A 46 <NA> -7.263 -7.635 9.274  
## 329 ATOM 329 CA <NA> GLY A 46 <NA> -7.720 -6.400 8.646  
## 330 ATOM 330 C <NA> GLY A 46 <NA> -7.338 -5.168 9.421  
## 331 ATOM 331 O <NA> GLY A 46 <NA> -7.028 -4.119 8.856  
## 332 ATOM 332 N <NA> LYS A 47 <NA> -7.381 -5.307 10.737  
## 333 ATOM 333 CA <NA> LYS A 47 <NA> -7.018 -4.236 11.637  
## 334 ATOM 334 C <NA> LYS A 47 <NA> -5.508 -4.052 11.520  
## 335 ATOM 335 O <NA> LYS A 47 <NA> -5.031 -2.925 11.418  
## 336 ATOM 336 CB <NA> LYS A 47 <NA> -7.391 -4.610 13.074  
## 337 ATOM 337 CG <NA> LYS A 47 <NA> -8.827 -5.132 13.273  
## 338 ATOM 338 CD <NA> LYS A 47 <NA> -9.840 -4.035 13.570  
## 339 ATOM 339 CE <NA> LYS A 47 <NA> -10.096 -3.117 12.383  
## 340 ATOM 340 NZ <NA> LYS A 47 <NA> -10.995 -1.993 12.789  
## 341 ATOM 341 N <NA> GLN A 48 <NA> -4.765 -5.164 11.506  
## 342 ATOM 342 CA <NA> GLN A 48 <NA> -3.304 -5.133 11.385  
## 343 ATOM 343 C <NA> GLN A 48 <NA> -2.917 -4.401 10.116  
## 344 ATOM 344 O <NA> GLN A 48 <NA> -2.051 -3.533 10.137  
## 345 ATOM 345 CB <NA> GLN A 48 <NA> -2.722 -6.553 11.345  
## 346 ATOM 346 CG <NA> GLN A 48 <NA> -2.593 -7.208 12.705  
## 347 ATOM 347 CD <NA> GLN A 48 <NA> -2.196 -8.673 12.645  
## 348 ATOM 348 OE1 <NA> GLN A 48 <NA> -1.031 -9.014 12.438  
## 349 ATOM 349 NE2 <NA> GLN A 48 <NA> -3.165 -9.548 12.858  
## 350 ATOM 350 N <NA> ALA A 49 <NA> -3.613 -4.714 9.030  
## 351 ATOM 351 CA <NA> ALA A 49 <NA> -3.366 -4.114 7.718  
## 352 ATOM 352 C <NA> ALA A 49 <NA> -3.857 -2.676 7.563  
## 353 ATOM 353 O <NA> ALA A 49 <NA> -3.302 -1.915 6.761  
## 354 ATOM 354 CB <NA> ALA A 49 <NA> -3.973 -4.981 6.632  
## 355 ATOM 355 N <NA> LYS A 50 <NA> -4.921 -2.320 8.284  
## 356 ATOM 356 CA <NA> LYS A 50 <NA> -5.455 -0.962 8.228  
## 357 ATOM 357 C <NA> LYS A 50 <NA> -4.451 0.026 8.809  
## 358 ATOM 358 O <NA> LYS A 50 <NA> -4.229 1.096 8.246  
## 359 ATOM 359 CB <NA> LYS A 50 <NA> -6.772 -0.858 8.981  
## 360 ATOM 360 CG <NA> LYS A 50 <NA> -7.296 0.548 9.059  
## 361 ATOM 361 CD <NA> LYS A 50 <NA> -8.631 0.593 9.767  
## 362 ATOM 362 CE <NA> LYS A 50 <NA> -9.003 2.007 10.225  
## 363 ATOM 363 NZ <NA> LYS A 50 <NA> -8.335 2.379 11.514  
## 364 ATOM 364 N <NA> ASP A 51 <NA> -3.843 -0.341 9.934  
## 365 ATOM 365 CA <NA> ASP A 51 <NA> -2.842 0.502 10.588  
## 366 ATOM 366 C <NA> ASP A 51 <NA> -1.627 0.707 9.707  
## 367 ATOM 367 O <NA> ASP A 51 <NA> -1.145 1.817 9.567  
## 368 ATOM 368 CB <NA> ASP A 51 <NA> -2.390 -0.104 11.922  
## 369 ATOM 369 CG <NA> ASP A 51 <NA> -3.425 0.057 13.023  
## 370 ATOM 370 OD1 <NA> ASP A 51 <NA> -3.719 1.214 13.417  
## 371 ATOM 371 OD2 <NA> ASP A 51 <NA> -3.930 -0.982 13.500  
## 372 ATOM 372 N <NA> ILE A 52 <NA> -1.118 -0.375 9.135  
## 373 ATOM 373 CA <NA> ILE A 52 <NA> 0.045 -0.309 8.254  
## 374 ATOM 374 C <NA> ILE A 52 <NA> -0.174 0.666 7.106  
## 375 ATOM 375 O <NA> ILE A 52 <NA> 0.651 1.538 6.882  
## 376 ATOM 376 CB <NA> ILE A 52 <NA> 0.419 -1.720 7.722  
## 377 ATOM 377 CG1 <NA> ILE A 52 <NA> 1.155 -2.494 8.817  
## 378 ATOM 378 CG2 <NA> ILE A 52 <NA> 1.261 -1.628 6.457  
## 379 ATOM 379 CD1 <NA> ILE A 52 <NA> 1.478 -3.889 8.438  
## 380 ATOM 380 N <NA> MET A 53 <NA> -1.283 0.505 6.392  
## 381 ATOM 381 CA <NA> MET A 53 <NA> -1.643 1.374 5.281  
## 382 ATOM 382 C <NA> MET A 53 <NA> -1.760 2.811 5.757  
## 383 ATOM 383 O <NA> MET A 53 <NA> -1.244 3.733 5.120  
## 384 ATOM 384 CB <NA> MET A 53 <NA> -3.012 1.010 4.758  
## 385 ATOM 385 CG <NA> MET A 53 <NA> -3.118 -0.228 3.941  
## 386 ATOM 386 SD <NA> MET A 53 <NA> -4.859 -0.224 3.434  
## 387 ATOM 387 CE <NA> MET A 53 <NA> -4.960 1.325 2.436  
## 388 ATOM 388 N <NA> ASP A 54 <NA> -2.531 2.991 6.828  
## 389 ATOM 389 CA <NA> ASP A 54 <NA> -2.778 4.300 7.444  
## 390 ATOM 390 C <NA> ASP A 54 <NA> -1.495 5.000 7.869  
## 391 ATOM 391 O <NA> ASP A 54 <NA> -1.418 6.228 7.825  
## 392 ATOM 392 CB <NA> ASP A 54 <NA> -3.704 4.174 8.667  
## 393 ATOM 393 CG <NA> ASP A 54 <NA> -5.158 3.935 8.289  
## 394 ATOM 394 OD1 <NA> ASP A 54 <NA> -5.433 3.561 7.129  
## 395 ATOM 395 OD2 <NA> ASP A 54 <NA> -6.026 4.124 9.167  
## 396 ATOM 396 N <NA> ALA A 55 <NA> -0.505 4.224 8.306  
## 397 ATOM 397 CA <NA> ALA A 55 <NA> 0.787 4.770 8.728  
## 398 ATOM 398 C <NA> ALA A 55 <NA> 1.707 4.959 7.530  
## 399 ATOM 399 O <NA> ALA A 55 <NA> 2.870 5.356 7.683  
## 400 ATOM 400 CB <NA> ALA A 55 <NA> 1.438 3.848 9.733  
## 401 ATOM 401 N <NA> GLY A 56 <NA> 1.181 4.654 6.344  
## 402 ATOM 402 CA <NA> GLY A 56 <NA> 1.935 4.782 5.112  
## 403 ATOM 403 C <NA> GLY A 56 <NA> 3.056 3.775 5.051  
## 404 ATOM 404 O <NA> GLY A 56 <NA> 4.089 4.041 4.440  
## 405 ATOM 405 N <NA> LYS A 57 <NA> 2.875 2.656 5.753  
## 406 ATOM 406 CA <NA> LYS A 57 <NA> 3.856 1.578 5.797  
## 407 ATOM 407 C <NA> LYS A 57 <NA> 3.436 0.536 4.783  
## 408 ATOM 408 O <NA> LYS A 57 <NA> 2.258 0.425 4.414  
## 409 ATOM 409 CB <NA> LYS A 57 <NA> 3.954 0.953 7.194  
## 410 ATOM 410 CG <NA> LYS A 57 <NA> 4.758 1.772 8.203  
## 411 ATOM 411 CD <NA> LYS A 57 <NA> 4.726 1.146 9.600  
## 412 ATOM 412 CE <NA> LYS A 57 <NA> 3.291 1.013 10.158  
## 413 ATOM 413 NZ <NA> LYS A 57 <NA> 3.199 0.297 11.484  
## 414 ATOM 414 N <NA> LEU A 58 <NA> 4.411 -0.233 4.332  
## 415 ATOM 415 CA <NA> LEU A 58 <NA> 4.156 -1.240 3.331  
## 416 ATOM 416 C <NA> LEU A 58 <NA> 3.811 -2.553 4.010  
## 417 ATOM 417 O <NA> LEU A 58 <NA> 4.354 -2.881 5.063  
## 418 ATOM 418 CB <NA> LEU A 58 <NA> 5.388 -1.350 2.429  
## 419 ATOM 419 CG <NA> LEU A 58 <NA> 5.291 -1.952 1.032  
## 420 ATOM 420 CD1 <NA> LEU A 58 <NA> 4.016 -1.505 0.294  
## 421 ATOM 421 CD2 <NA> LEU A 58 <NA> 6.545 -1.541 0.293  
## 422 ATOM 422 N <NA> VAL A 59 <NA> 2.833 -3.244 3.441  
## 423 ATOM 423 CA <NA> VAL A 59 <NA> 2.365 -4.528 3.951  
## 424 ATOM 424 C <NA> VAL A 59 <NA> 3.391 -5.614 3.689  
## 425 ATOM 425 O <NA> VAL A 59 <NA> 3.815 -5.824 2.555  
## 426 ATOM 426 CB <NA> VAL A 59 <NA> 1.038 -4.958 3.272  
## 427 ATOM 427 CG1 <NA> VAL A 59 <NA> 0.553 -6.298 3.842  
## 428 ATOM 428 CG2 <NA> VAL A 59 <NA> -0.018 -3.866 3.440  
## 429 ATOM 429 N <NA> THR A 60 <NA> 3.760 -6.334 4.730  
## 430 ATOM 430 CA <NA> THR A 60 <NA> 4.734 -7.387 4.575  
## 431 ATOM 431 C <NA> THR A 60 <NA> 4.162 -8.657 3.918  
## 432 ATOM 432 O <NA> THR A 60 <NA> 2.963 -8.942 4.000  
## 433 ATOM 433 CB <NA> THR A 60 <NA> 5.351 -7.685 5.918  
## 434 ATOM 434 OG1 <NA> THR A 60 <NA> 4.310 -7.899 6.883  
## 435 ATOM 435 CG2 <NA> THR A 60 <NA> 6.181 -6.502 6.350  
## 436 ATOM 436 N <NA> ASP A 61 <NA> 5.025 -9.410 3.247  
## 437 ATOM 437 CA <NA> ASP A 61 <NA> 4.606 -10.636 2.574  
## 438 ATOM 438 C <NA> ASP A 61 <NA> 3.810 -11.495 3.516  
## 439 ATOM 439 O <NA> ASP A 61 <NA> 2.831 -12.130 3.145  
## 440 ATOM 440 CB <NA> ASP A 61 <NA> 5.820 -11.460 2.149  
## 441 ATOM 441 CG <NA> ASP A 61 <NA> 6.623 -10.810 1.062  
## 442 ATOM 442 OD1 <NA> ASP A 61 <NA> 6.131 -9.825 0.464  
## 443 ATOM 443 OD2 <NA> ASP A 61 <NA> 7.744 -11.306 0.805  
## 444 ATOM 444 N <NA> GLU A 62 <NA> 4.269 -11.502 4.751  
## 445 ATOM 445 CA <NA> GLU A 62 <NA> 3.685 -12.298 5.799  
## 446 ATOM 446 C <NA> GLU A 62 <NA> 2.225 -11.992 6.029  
## 447 ATOM 447 O <NA> GLU A 62 <NA> 1.407 -12.907 6.137  
## 448 ATOM 448 CB <NA> GLU A 62 <NA> 4.506 -12.112 7.072  
## 449 ATOM 449 CG <NA> GLU A 62 <NA> 5.984 -12.590 6.943  
## 450 ATOM 450 CD <NA> GLU A 62 <NA> 6.903 -11.648 6.144  
## 451 ATOM 451 OE1 <NA> GLU A 62 <NA> 6.867 -10.424 6.394  
## 452 ATOM 452 OE2 <NA> GLU A 62 <NA> 7.682 -12.138 5.288  
## 453 ATOM 453 N <NA> LEU A 63 <NA> 1.901 -10.707 6.064  
## 454 ATOM 454 CA <NA> LEU A 63 <NA> 0.529 -10.257 6.268  
## 455 ATOM 455 C <NA> LEU A 63 <NA> -0.256 -10.493 4.986  
## 456 ATOM 456 O <NA> LEU A 63 <NA> -1.432 -10.857 5.031  
## 457 ATOM 457 CB <NA> LEU A 63 <NA> 0.509 -8.784 6.658  
## 458 ATOM 458 CG <NA> LEU A 63 <NA> -0.605 -8.296 7.574  
## 459 ATOM 459 CD1 <NA> LEU A 63 <NA> -0.221 -6.936 8.069  
## 460 ATOM 460 CD2 <NA> LEU A 63 <NA> -1.931 -8.226 6.850  
## 461 ATOM 461 N <NA> VAL A 64 <NA> 0.397 -10.331 3.842  
## 462 ATOM 462 CA <NA> VAL A 64 <NA> -0.278 -10.586 2.587  
## 463 ATOM 463 C <NA> VAL A 64 <NA> -0.674 -12.043 2.451  
## 464 ATOM 464 O <NA> VAL A 64 <NA> -1.797 -12.326 2.067  
## 465 ATOM 465 CB <NA> VAL A 64 <NA> 0.561 -10.248 1.381  
## 466 ATOM 466 CG1 <NA> VAL A 64 <NA> -0.296 -10.350 0.124  
## 467 ATOM 467 CG2 <NA> VAL A 64 <NA> 1.111 -8.875 1.525  
## 468 ATOM 468 N <NA> ILE A 65 <NA> 0.225 -12.977 2.748  
## 469 ATOM 469 CA <NA> ILE A 65 <NA> -0.115 -14.401 2.626  
## 470 ATOM 470 C <NA> ILE A 65 <NA> -1.234 -14.782 3.573  
## 471 ATOM 471 O <NA> ILE A 65 <NA> -2.061 -15.648 3.255  
## 472 ATOM 472 CB <NA> ILE A 65 <NA> 1.124 -15.356 2.772  
## 473 ATOM 473 CG1 <NA> ILE A 65 <NA> 1.655 -15.751 1.390  
## 474 ATOM 474 CG2 <NA> ILE A 65 <NA> 0.734 -16.675 3.418  
## 475 ATOM 475 CD1 <NA> ILE A 65 <NA> 2.201 -14.615 0.586  
## 476 ATOM 476 N <NA> ALA A 66 <NA> -1.275 -14.102 4.718  
## 477 ATOM 477 CA <NA> ALA A 66 <NA> -2.297 -14.315 5.740  
## 478 ATOM 478 C <NA> ALA A 66 <NA> -3.685 -13.867 5.237  
## 479 ATOM 479 O <NA> ALA A 66 <NA> -4.700 -14.517 5.523  
## 480 ATOM 480 CB <NA> ALA A 66 <NA> -1.922 -13.562 6.983  
## 481 ATOM 481 N <NA> LEU A 67 <NA> -3.725 -12.763 4.489  
## 482 ATOM 482 CA <NA> LEU A 67 <NA> -4.978 -12.266 3.939  
## 483 ATOM 483 C <NA> LEU A 67 <NA> -5.460 -13.165 2.833  
## 484 ATOM 484 O <NA> LEU A 67 <NA> -6.653 -13.297 2.644  
## 485 ATOM 485 CB <NA> LEU A 67 <NA> -4.832 -10.866 3.366  
## 486 ATOM 486 CG <NA> LEU A 67 <NA> -4.395 -9.691 4.227  
## 487 ATOM 487 CD1 <NA> LEU A 67 <NA> -4.558 -8.468 3.362  
## 488 ATOM 488 CD2 <NA> LEU A 67 <NA> -5.226 -9.569 5.501  
## 489 ATOM 489 N <NA> VAL A 68 <NA> -4.534 -13.774 2.097  
## 490 ATOM 490 CA <NA> VAL A 68 <NA> -4.880 -14.670 0.987  
## 491 ATOM 491 C <NA> VAL A 68 <NA> -5.419 -15.970 1.546  
## 492 ATOM 492 O <NA> VAL A 68 <NA> -6.321 -16.567 0.967  
## 493 ATOM 493 CB <NA> VAL A 68 <NA> -3.649 -15.001 0.041  
## 494 ATOM 494 CG1 <NA> VAL A 68 <NA> -4.036 -16.018 -1.022  
## 495 ATOM 495 CG2 <NA> VAL A 68 <NA> -3.093 -13.752 -0.641  
## 496 ATOM 496 N <NA> LYS A 69 <NA> -4.876 -16.420 2.671  
## 497 ATOM 497 CA <NA> LYS A 69 <NA> -5.342 -17.671 3.275  
## 498 ATOM 498 C <NA> LYS A 69 <NA> -6.732 -17.449 3.875  
## 499 ATOM 499 O <NA> LYS A 69 <NA> -7.621 -18.294 3.750  
## 500 ATOM 500 CB <NA> LYS A 69 <NA> -4.342 -18.142 4.321  
## 501 ATOM 501 CG <NA> LYS A 69 <NA> -4.326 -19.631 4.531  
## 502 ATOM 502 CD <NA> LYS A 69 <NA> -3.018 -20.052 5.189  
## 503 ATOM 503 CE <NA> LYS A 69 <NA> -2.716 -19.271 6.489  
## 504 ATOM 504 NZ <NA> LYS A 69 <NA> -1.350 -19.533 7.084  
## 505 ATOM 505 N <NA> GLU A 70 <NA> -6.912 -16.286 4.494  
## 506 ATOM 506 CA <NA> GLU A 70 <NA> -8.182 -15.890 5.071  
## 507 ATOM 507 C <NA> GLU A 70 <NA> -9.199 -15.792 3.922  
## 508 ATOM 508 O <NA> GLU A 70 <NA> -10.213 -16.489 3.900  
## 509 ATOM 509 CB <NA> GLU A 70 <NA> -8.017 -14.518 5.740  
## 510 ATOM 510 CG <NA> GLU A 70 <NA> -9.313 -13.846 6.198  
## 511 ATOM 511 CD <NA> GLU A 70 <NA> -9.104 -12.459 6.815  
## 512 ATOM 512 OE1 <NA> GLU A 70 <NA> -8.294 -12.340 7.760  
## 513 ATOM 513 OE2 <NA> GLU A 70 <NA> -9.759 -11.487 6.367  
## 514 ATOM 514 N <NA> ARG A 71 <NA> -8.878 -14.966 2.933  
## 515 ATOM 515 CA <NA> ARG A 71 <NA> -9.735 -14.749 1.788  
## 516 ATOM 516 C <NA> ARG A 71 <NA> -10.196 -15.995 1.081  
## 517 ATOM 517 O <NA> ARG A 71 <NA> -11.393 -16.209 0.943  
## 518 ATOM 518 CB <NA> ARG A 71 <NA> -9.049 -13.848 0.761  
## 519 ATOM 519 CG <NA> ARG A 71 <NA> -9.901 -13.566 -0.476  
## 520 ATOM 520 CD <NA> ARG A 71 <NA> -11.097 -12.676 -0.128  
## 521 ATOM 521 NE <NA> ARG A 71 <NA> -11.989 -12.489 -1.266  
## 522 ATOM 522 CZ <NA> ARG A 71 <NA> -12.837 -13.404 -1.713  
## 523 ATOM 523 NH1 <NA> ARG A 71 <NA> -12.950 -14.570 -1.101  
## 524 ATOM 524 NH2 <NA> ARG A 71 <NA> -13.596 -13.143 -2.763  
## 525 ATOM 525 N <NA> ILE A 72 <NA> -9.268 -16.820 0.618  
## 526 ATOM 526 CA <NA> ILE A 72 <NA> -9.664 -18.002 -0.136  
## 527 ATOM 527 C <NA> ILE A 72 <NA> -10.391 -19.024 0.700  
## 528 ATOM 528 O <NA> ILE A 72 <NA> -10.702 -20.110 0.229  
## 529 ATOM 529 CB <NA> ILE A 72 <NA> -8.486 -18.639 -0.878  
## 530 ATOM 530 CG1 <NA> ILE A 72 <NA> -7.518 -19.277 0.112  
## 531 ATOM 531 CG2 <NA> ILE A 72 <NA> -7.787 -17.577 -1.728  
## 532 ATOM 532 CD1 <NA> ILE A 72 <NA> -6.322 -19.871 -0.538  
## 533 ATOM 533 N <NA> ALA A 73 <NA> -10.586 -18.695 1.970  
## 534 ATOM 534 CA <NA> ALA A 73 <NA> -11.326 -19.542 2.895  
## 535 ATOM 535 C <NA> ALA A 73 <NA> -12.815 -19.149 2.819  
## 536 ATOM 536 O <NA> ALA A 73 <NA> -13.678 -19.834 3.379  
## 537 ATOM 537 CB <NA> ALA A 73 <NA> -10.803 -19.373 4.311  
## 538 ATOM 538 N <NA> GLN A 74 <NA> -13.106 -18.019 2.173  
## 539 ATOM 539 CA <NA> GLN A 74 <NA> -14.475 -17.584 1.995  
## 540 ATOM 540 C <NA> GLN A 74 <NA> -15.129 -18.583 1.045  
## 541 ATOM 541 O <NA> GLN A 74 <NA> -14.466 -19.197 0.209  
## 542 ATOM 542 CB <NA> GLN A 74 <NA> -14.526 -16.161 1.484  
## 543 ATOM 543 CG <NA> GLN A 74 <NA> -13.977 -15.201 2.512  
## 544 ATOM 544 CD <NA> GLN A 74 <NA> -14.017 -13.741 2.077  
## 545 ATOM 545 OE1 <NA> GLN A 74 <NA> -13.417 -12.878 2.724  
## 546 ATOM 546 NE2 <NA> GLN A 74 <NA> -14.727 -13.452 0.987  
## 547 ATOM 547 N <NA> GLU A 75 <NA> -16.427 -18.775 1.223  
## 548 ATOM 548 CA <NA> GLU A 75 <NA> -17.200 -19.754 0.468  
## 549 ATOM 549 C <NA> GLU A 75 <NA> -17.335 -19.505 -1.028  
## 550 ATOM 550 O <NA> GLU A 75 <NA> -17.616 -20.435 -1.802  
## 551 ATOM 551 CB <NA> GLU A 75 <NA> -18.569 -19.931 1.139  
## 552 ATOM 552 CG <NA> GLU A 75 <NA> -18.474 -20.343 2.634  
## 553 ATOM 553 CD <NA> GLU A 75 <NA> -19.090 -19.320 3.595  
## 554 ATOM 554 OE1 <NA> GLU A 75 <NA> -18.635 -18.147 3.628  
## 555 ATOM 555 OE2 <NA> GLU A 75 <NA> -20.030 -19.701 4.328  
## 556 ATOM 556 N <NA> ASP A 76 <NA> -17.124 -18.251 -1.429  
## 557 ATOM 557 CA <NA> ASP A 76 <NA> -17.185 -17.880 -2.839  
## 558 ATOM 558 C <NA> ASP A 76 <NA> -15.974 -18.428 -3.616  
## 559 ATOM 559 O <NA> ASP A 76 <NA> -15.989 -18.467 -4.854  
## 560 ATOM 560 CB <NA> ASP A 76 <NA> -17.379 -16.360 -3.028  
## 561 ATOM 561 CG <NA> ASP A 76 <NA> -16.169 -15.533 -2.651  
## 562 ATOM 562 OD1 <NA> ASP A 76 <NA> -15.299 -16.002 -1.907  
## 563 ATOM 563 OD2 <NA> ASP A 76 <NA> -16.100 -14.375 -3.107  
## 564 ATOM 564 N <NA> CYS A 77 <NA> -14.960 -18.897 -2.877  
## 565 ATOM 565 CA <NA> CYS A 77 <NA> -13.764 -19.497 -3.470  
## 566 ATOM 566 C <NA> CYS A 77 <NA> -13.861 -21.002 -3.330  
## 567 ATOM 567 O <NA> CYS A 77 <NA> -12.851 -21.703 -3.328  
## 568 ATOM 568 CB <NA> CYS A 77 <NA> -12.502 -19.027 -2.765  
## 569 ATOM 569 SG <NA> CYS A 77 <NA> -12.229 -17.284 -2.859  
## 570 ATOM 570 N <NA> ARG A 78 <NA> -15.079 -21.502 -3.179  
## 571 ATOM 571 CA <NA> ARG A 78 <NA> -15.293 -22.933 -3.019  
## 572 ATOM 572 C <NA> ARG A 78 <NA> -14.995 -23.694 -4.310  
## 573 ATOM 573 O <NA> ARG A 78 <NA> -14.730 -24.896 -4.269  
## 574 ATOM 574 CB <NA> ARG A 78 <NA> -16.722 -23.179 -2.530  
## 575 ATOM 575 CG <NA> ARG A 78 <NA> -17.100 -24.628 -2.259  
## 576 ATOM 576 CD <NA> ARG A 78 <NA> -18.494 -24.740 -1.607  
## 577 ATOM 577 NE <NA> ARG A 78 <NA> -18.434 -25.043 -0.172  
## 578 ATOM 578 CZ <NA> ARG A 78 <NA> -18.109 -24.167 0.781  
## 579 ATOM 579 NH1 <NA> ARG A 78 <NA> -17.827 -22.907 0.469  
## 580 ATOM 580 NH2 <NA> ARG A 78 <NA> -18.082 -24.551 2.053  
## 581 ATOM 581 N <NA> ASN A 79 <NA> -14.994 -22.988 -5.447  
## 582 ATOM 582 CA <NA> ASN A 79 <NA> -14.722 -23.611 -6.752  
## 583 ATOM 583 C <NA> ASN A 79 <NA> -13.300 -23.366 -7.236  
## 584 ATOM 584 O <NA> ASN A 79 <NA> -12.859 -23.924 -8.236  
## 585 ATOM 585 CB <NA> ASN A 79 <NA> -15.694 -23.098 -7.811  
## 586 ATOM 586 CG <NA> ASN A 79 <NA> -17.134 -23.479 -7.525  
## 587 ATOM 587 OD1 <NA> ASN A 79 <NA> -17.501 -24.650 -7.589  
## 588 ATOM 588 ND2 <NA> ASN A 79 <NA> -17.963 -22.482 -7.234  
## 589 ATOM 589 N <NA> GLY A 80 <NA> -12.593 -22.506 -6.525  
## 590 ATOM 590 CA <NA> GLY A 80 <NA> -11.233 -22.180 -6.869  
## 591 ATOM 591 C <NA> GLY A 80 <NA> -11.157 -20.677 -6.854  
## 592 ATOM 592 O <NA> GLY A 80 <NA> -11.969 -20.005 -6.206  
## 593 ATOM 593 N <NA> PHE A 81 <NA> -10.239 -20.129 -7.628  
## 594 ATOM 594 CA <NA> PHE A 81 <NA> -10.086 -18.686 -7.664  
## 595 ATOM 595 C <NA> PHE A 81 <NA> -9.076 -18.251 -8.718  
## 596 ATOM 596 O <NA> PHE A 81 <NA> -8.280 -19.066 -9.186  
## 597 ATOM 597 CB <NA> PHE A 81 <NA> -9.692 -18.157 -6.275  
## 598 ATOM 598 CG <NA> PHE A 81 <NA> -8.501 -18.869 -5.645  
## 599 ATOM 599 CD1 <NA> PHE A 81 <NA> -7.199 -18.586 -6.059  
## 600 ATOM 600 CD2 <NA> PHE A 81 <NA> -8.687 -19.781 -4.598  
## 601 ATOM 601 CE1 <NA> PHE A 81 <NA> -6.105 -19.194 -5.440  
## 602 ATOM 602 CE2 <NA> PHE A 81 <NA> -7.607 -20.386 -3.978  
## 603 ATOM 603 CZ <NA> PHE A 81 <NA> -6.312 -20.097 -4.396  
## 604 ATOM 604 N <NA> LEU A 82 <NA> -9.150 -16.980 -9.112  
## 605 ATOM 605 CA <NA> LEU A 82 <NA> -8.252 -16.401 -10.097  
## 606 ATOM 606 C <NA> LEU A 82 <NA> -7.502 -15.317 -9.375  
## 607 ATOM 607 O <NA> LEU A 82 <NA> -8.066 -14.298 -9.018  
## 608 ATOM 608 CB <NA> LEU A 82 <NA> -9.026 -15.798 -11.273  
## 609 ATOM 609 CG <NA> LEU A 82 <NA> -8.299 -15.043 -12.386  
## 610 ATOM 610 CD1 <NA> LEU A 82 <NA> -7.291 -15.935 -13.096  
## 611 ATOM 611 CD2 <NA> LEU A 82 <NA> -9.336 -14.557 -13.376  
## 612 ATOM 612 N <NA> LEU A 83 <NA> -6.247 -15.610 -9.077  
## 613 ATOM 613 CA <NA> LEU A 83 <NA> -5.348 -14.700 -8.398  
## 614 ATOM 614 C <NA> LEU A 83 <NA> -4.661 -13.917 -9.523  
## 615 ATOM 615 O <NA> LEU A 83 <NA> -3.934 -14.455 -10.362  
## 616 ATOM 616 CB <NA> LEU A 83 <NA> -4.371 -15.520 -7.551  
## 617 ATOM 617 CG <NA> LEU A 83 <NA> -3.488 -14.850 -6.517  
## 618 ATOM 618 CD1 <NA> LEU A 83 <NA> -4.285 -13.921 -5.611  
## 619 ATOM 619 CD2 <NA> LEU A 83 <NA> -2.822 -15.949 -5.732  
## 620 ATOM 620 N <NA> ASP A 84 <NA> -4.938 -12.634 -9.551  
## 621 ATOM 621 CA <NA> ASP A 84 <NA> -4.443 -11.758 -10.590  
## 622 ATOM 622 C <NA> ASP A 84 <NA> -3.178 -11.011 -10.155  
## 623 ATOM 623 O <NA> ASP A 84 <NA> -3.237 -10.195 -9.246  
## 624 ATOM 624 CB <NA> ASP A 84 <NA> -5.602 -10.799 -10.929  
## 625 ATOM 625 CG <NA> ASP A 84 <NA> -5.197 -9.652 -11.811  
## 626 ATOM 626 OD1 <NA> ASP A 84 <NA> -5.003 -9.859 -13.021  
## 627 ATOM 627 OD2 <NA> ASP A 84 <NA> -5.125 -8.519 -11.300  
## 628 ATOM 628 N <NA> GLY A 85 <NA> -2.033 -11.320 -10.770  
## 629 ATOM 629 CA <NA> GLY A 85 <NA> -0.781 -10.634 -10.440  
## 630 ATOM 630 C <NA> GLY A 85 <NA> -0.128 -10.839 -9.076  
## 631 ATOM 631 O <NA> GLY A 85 <NA> 0.513 -9.917 -8.536  
## 632 ATOM 632 N <NA> PHE A 86 <NA> -0.348 -12.006 -8.470  
## 633 ATOM 633 CA <NA> PHE A 86 <NA> 0.255 -12.328 -7.186  
## 634 ATOM 634 C <NA> PHE A 86 <NA> 0.346 -13.824 -7.150  
## 635 ATOM 635 O <NA> PHE A 86 <NA> -0.638 -14.491 -7.401  
## 636 ATOM 636 CB <NA> PHE A 86 <NA> -0.578 -11.865 -6.000  
## 637 ATOM 637 CG <NA> PHE A 86 <NA> 0.085 -12.155 -4.668  
## 638 ATOM 638 CD1 <NA> PHE A 86 <NA> 1.052 -11.301 -4.155  
## 639 ATOM 639 CD2 <NA> PHE A 86 <NA> -0.157 -13.345 -3.993  
## 640 ATOM 640 CE1 <NA> PHE A 86 <NA> 1.765 -11.637 -3.008  
## 641 ATOM 641 CE2 <NA> PHE A 86 <NA> 0.563 -13.672 -2.847  
## 642 ATOM 642 CZ <NA> PHE A 86 <NA> 1.516 -12.825 -2.365  
## 643 ATOM 643 N <NA> PRO A 87 <NA> 1.497 -14.371 -6.734  
## 644 ATOM 644 CA <NA> PRO A 87 <NA> 2.733 -13.731 -6.277  
## 645 ATOM 645 C <NA> PRO A 87 <NA> 3.529 -12.859 -7.243  
## 646 ATOM 646 O <NA> PRO A 87 <NA> 3.362 -12.940 -8.445  
## 647 ATOM 647 CB <NA> PRO A 87 <NA> 3.566 -14.926 -5.825  
## 648 ATOM 648 CG <NA> PRO A 87 <NA> 3.097 -16.003 -6.662  
## 649 ATOM 649 CD <NA> PRO A 87 <NA> 1.621 -15.826 -6.597  
## 650 ATOM 650 N <NA> ARG A 88 <NA> 4.370 -11.993 -6.690  
## 651 ATOM 651 CA <NA> ARG A 88 <NA> 5.248 -11.143 -7.479  
## 652 ATOM 652 C <NA> ARG A 88 <NA> 6.734 -11.526 -7.331  
## 653 ATOM 653 O <NA> ARG A 88 <NA> 7.593 -11.006 -8.044  
## 654 ATOM 654 CB <NA> ARG A 88 <NA> 5.080 -9.700 -7.072  
## 655 ATOM 655 CG <NA> ARG A 88 <NA> 3.808 -9.115 -7.543  
## 656 ATOM 656 CD <NA> ARG A 88 <NA> 3.632 -7.743 -7.000  
## 657 ATOM 657 NE <NA> ARG A 88 <NA> 2.337 -7.676 -6.329  
## 658 ATOM 658 CZ <NA> ARG A 88 <NA> 2.174 -7.566 -5.009  
## 659 ATOM 659 NH1 <NA> ARG A 88 <NA> 3.233 -7.457 -4.211  
## 660 ATOM 660 NH2 <NA> ARG A 88 <NA> 0.947 -7.522 -4.489  
## 661 ATOM 661 N <NA> THR A 89 <NA> 7.042 -12.443 -6.414  
## 662 ATOM 662 CA <NA> THR A 89 <NA> 8.423 -12.849 -6.179  
## 663 ATOM 663 C <NA> THR A 89 <NA> 8.469 -14.304 -5.725  
## 664 ATOM 664 O <NA> THR A 89 <NA> 7.450 -14.826 -5.270  
## 665 ATOM 665 CB <NA> THR A 89 <NA> 9.018 -12.014 -5.046  
## 666 ATOM 666 OG1 <NA> THR A 89 <NA> 8.308 -12.308 -3.842  
## 667 ATOM 667 CG2 <NA> THR A 89 <NA> 8.890 -10.535 -5.326  
## 668 ATOM 668 N <NA> ILE A 90 <NA> 9.643 -14.947 -5.829  
## 669 ATOM 669 CA <NA> ILE A 90 <NA> 9.848 -16.353 -5.387  
## 670 ATOM 670 C <NA> ILE A 90 <NA> 9.563 -16.476 -3.899  
## 671 ATOM 671 O <NA> ILE A 90 <NA> 9.058 -17.497 -3.452  
## 672 ATOM 672 CB <NA> ILE A 90 <NA> 11.292 -16.877 -5.667  
## 673 ATOM 673 CG1 <NA> ILE A 90 <NA> 11.481 -17.118 -7.167  
## 674 ATOM 674 CG2 <NA> ILE A 90 <NA> 11.574 -18.178 -4.855  
## 675 ATOM 675 CD1 <NA> ILE A 90 <NA> 12.916 -17.320 -7.596  
## 676 ATOM 676 N <NA> PRO A 91 <NA> 9.982 -15.478 -3.102  
## 677 ATOM 677 CA <NA> PRO A 91 <NA> 9.733 -15.505 -1.668  
## 678 ATOM 678 C <NA> PRO A 91 <NA> 8.248 -15.565 -1.402  
## 679 ATOM 679 O <NA> PRO A 91 <NA> 7.830 -16.255 -0.485  
## 680 ATOM 680 CB <NA> PRO A 91 <NA> 10.304 -14.183 -1.218  
## 681 ATOM 681 CG <NA> PRO A 91 <NA> 11.508 -14.075 -2.055  
## 682 ATOM 682 CD <NA> PRO A 91 <NA> 10.943 -14.403 -3.408  
## 683 ATOM 683 N <NA> GLN A 92 <NA> 7.455 -14.821 -2.175  
## 684 ATOM 684 CA <NA> GLN A 92 <NA> 5.989 -14.839 -2.027  
## 685 ATOM 685 C <NA> GLN A 92 <NA> 5.370 -16.146 -2.508  
## 686 ATOM 686 O <NA> GLN A 92 <NA> 4.463 -16.686 -1.881  
## 687 ATOM 687 CB <NA> GLN A 92 <NA> 5.374 -13.699 -2.800  
## 688 ATOM 688 CG <NA> GLN A 92 <NA> 5.490 -12.400 -2.062  
## 689 ATOM 689 CD <NA> GLN A 92 <NA> 5.209 -11.201 -2.920  
## 690 ATOM 690 OE1 <NA> GLN A 92 <NA> 5.181 -10.077 -2.428  
## 691 ATOM 691 NE2 <NA> GLN A 92 <NA> 5.067 -11.416 -4.222  
## 692 ATOM 692 N <NA> ALA A 93 <NA> 5.895 -16.672 -3.609  
## 693 ATOM 693 CA <NA> ALA A 93 <NA> 5.415 -17.915 -4.186  
## 694 ATOM 694 C <NA> ALA A 93 <NA> 5.724 -19.099 -3.289  
## 695 ATOM 695 O <NA> ALA A 93 <NA> 4.922 -20.004 -3.127  
## 696 ATOM 696 CB <NA> ALA A 93 <NA> 6.049 -18.119 -5.566  
## 697 ATOM 697 N <NA> ASP A 94 <NA> 6.912 -19.096 -2.723  
## 698 ATOM 698 CA <NA> ASP A 94 <NA> 7.335 -20.175 -1.866  
## 699 ATOM 699 C <NA> ASP A 94 <NA> 6.493 -20.235 -0.600  
## 700 ATOM 700 O <NA> ASP A 94 <NA> 6.163 -21.315 -0.132  
## 701 ATOM 701 CB <NA> ASP A 94 <NA> 8.814 -20.013 -1.540  
## 702 ATOM 702 CG <NA> ASP A 94 <NA> 9.487 -21.331 -1.326  
## 703 ATOM 703 OD1 <NA> ASP A 94 <NA> 9.729 -22.033 -2.331  
## 704 ATOM 704 OD2 <NA> ASP A 94 <NA> 9.728 -21.685 -0.153  
## 705 ATOM 705 N <NA> ALA A 95 <NA> 6.127 -19.072 -0.067  
## 706 ATOM 706 CA <NA> ALA A 95 <NA> 5.301 -18.979 1.142  
## 707 ATOM 707 C <NA> ALA A 95 <NA> 3.908 -19.507 0.887  
## 708 ATOM 708 O <NA> ALA A 95 <NA> 3.321 -20.141 1.751  
## 709 ATOM 709 CB <NA> ALA A 95 <NA> 5.225 -17.562 1.644  
## 710 ATOM 710 N <NA> MET A 96 <NA> 3.366 -19.245 -0.292  
## 711 ATOM 711 CA <NA> MET A 96 <NA> 2.051 -19.767 -0.607  
## 712 ATOM 712 C <NA> MET A 96 <NA> 2.112 -21.264 -0.564  
## 713 ATOM 713 O <NA> MET A 96 <NA> 1.181 -21.899 -0.097  
## 714 ATOM 714 CB <NA> MET A 96 <NA> 1.603 -19.350 -1.996  
## 715 ATOM 715 CG <NA> MET A 96 <NA> 0.961 -18.000 -2.012  
## 716 ATOM 716 SD <NA> MET A 96 <NA> 0.720 -17.544 -3.700  
## 717 ATOM 717 CE <NA> MET A 96 <NA> -0.855 -18.271 -4.003  
## 718 ATOM 718 N <NA> LYS A 97 <NA> 3.198 -21.839 -1.059  
## 719 ATOM 719 CA <NA> LYS A 97 <NA> 3.301 -23.289 -1.077  
## 720 ATOM 720 C <NA> LYS A 97 <NA> 3.358 -23.845 0.332  
## 721 ATOM 721 O <NA> LYS A 97 <NA> 2.708 -24.848 0.632  
## 722 ATOM 722 CB <NA> LYS A 97 <NA> 4.528 -23.758 -1.868  
## 723 ATOM 723 CG <NA> LYS A 97 <NA> 4.538 -25.279 -2.059  
## 724 ATOM 724 CD <NA> LYS A 97 <NA> 5.473 -25.769 -3.159  
## 725 ATOM 725 CE <NA> LYS A 97 <NA> 6.919 -25.770 -2.739  
## 726 ATOM 726 NZ <NA> LYS A 97 <NA> 7.701 -26.651 -3.655  
## 727 ATOM 727 N <NA> GLU A 98 <NA> 4.131 -23.168 1.182  
## 728 ATOM 728 CA <NA> GLU A 98 <NA> 4.337 -23.551 2.575  
## 729 ATOM 729 C <NA> GLU A 98 <NA> 3.073 -23.465 3.401  
## 730 ATOM 730 O <NA> GLU A 98 <NA> 2.905 -24.216 4.359  
## 731 ATOM 731 CB <NA> GLU A 98 <NA> 5.436 -22.698 3.206  
## 732 ATOM 732 CG <NA> GLU A 98 <NA> 6.795 -22.816 2.520  
## 733 ATOM 733 CD <NA> GLU A 98 <NA> 7.554 -24.071 2.911  
## 734 ATOM 734 OE1 <NA> GLU A 98 <NA> 7.983 -24.146 4.087  
## 735 ATOM 735 OE2 <NA> GLU A 98 <NA> 7.733 -24.971 2.047  
## 736 ATOM 736 N <NA> ALA A 99 <NA> 2.197 -22.529 3.058  
## 737 ATOM 737 CA <NA> ALA A 99 <NA> 0.921 -22.393 3.754  
## 738 ATOM 738 C <NA> ALA A 99 <NA> -0.123 -23.395 3.234  
## 739 ATOM 739 O <NA> ALA A 99 <NA> -1.263 -23.397 3.704  
## 740 ATOM 740 CB <NA> ALA A 99 <NA> 0.393 -20.971 3.639  
## 741 ATOM 741 N <NA> GLY A 100 <NA> 0.266 -24.217 2.250  
## 742 ATOM 742 CA <NA> GLY A 100 <NA> -0.621 -25.227 1.679  
## 743 ATOM 743 C <NA> GLY A 100 <NA> -1.509 -24.747 0.545  
## 744 ATOM 744 O <NA> GLY A 100 <NA> -2.408 -25.457 0.119  
## 745 ATOM 745 N <NA> ILE A 101 <NA> -1.248 -23.549 0.046  
## 746 ATOM 746 CA <NA> ILE A 101 <NA> -2.019 -22.965 -1.036  
## 747 ATOM 747 C <NA> ILE A 101 <NA> -1.484 -23.407 -2.397  
## 748 ATOM 748 O <NA> ILE A 101 <NA> -0.587 -22.783 -2.947  
## 749 ATOM 749 CB <NA> ILE A 101 <NA> -1.952 -21.438 -0.950  
## 750 ATOM 750 CG1 <NA> ILE A 101 <NA> -2.504 -20.971 0.394  
## 751 ATOM 751 CG2 <NA> ILE A 101 <NA> -2.757 -20.815 -2.065  
## 752 ATOM 752 CD1 <NA> ILE A 101 <NA> -2.301 -19.507 0.665  
## 753 ATOM 753 N <NA> ASN A 102 <NA> -1.995 -24.501 -2.928  
## 754 ATOM 754 CA <NA> ASN A 102 <NA> -1.521 -24.964 -4.218  
## 755 ATOM 755 C <NA> ASN A 102 <NA> -2.342 -24.299 -5.311  
## 756 ATOM 756 O <NA> ASN A 102 <NA> -3.386 -23.727 -5.024  
## 757 ATOM 757 CB <NA> ASN A 102 <NA> -1.652 -26.481 -4.319  
## 758 ATOM 758 CG <NA> ASN A 102 <NA> -3.080 -26.931 -4.235  
## 759 ATOM 759 OD1 <NA> ASN A 102 <NA> -3.741 -26.688 -3.228  
## 760 ATOM 760 ND2 <NA> ASN A 102 <NA> -3.587 -27.559 -5.301  
## 761 ATOM 761 N <NA> VAL A 103 <NA> -1.848 -24.340 -6.552  
## 762 ATOM 762 CA <NA> VAL A 103 <NA> -2.549 -23.751 -7.701  
## 763 ATOM 763 C <NA> VAL A 103 <NA> -2.460 -24.693 -8.864  
## 764 ATOM 764 O <NA> VAL A 103 <NA> -1.428 -25.251 -9.138  
## 765 ATOM 765 CB <NA> VAL A 103 <NA> -1.987 -22.367 -8.166  
## 766 ATOM 766 CG1 <NA> VAL A 103 <NA> -2.159 -21.336 -7.090  
## 767 ATOM 767 CG2 <NA> VAL A 103 <NA> -0.546 -22.458 -8.575  
## 768 ATOM 768 N <NA> ASP A 104 <NA> -3.549 -24.871 -9.570  
## 769 ATOM 769 CA <NA> ASP A 104 <NA> -3.511 -25.770 -10.690  
## 770 ATOM 770 C <NA> ASP A 104 <NA> -2.793 -25.183 -11.873  
## 771 ATOM 771 O <NA> ASP A 104 <NA> -2.163 -25.923 -12.613  
## 772 ATOM 772 CB <NA> ASP A 104 <NA> -4.927 -26.120 -11.113  
## 773 ATOM 773 CG <NA> ASP A 104 <NA> -5.708 -26.712 -10.012  
## 774 ATOM 774 OD1 <NA> ASP A 104 <NA> -5.427 -27.881 -9.675  
## 775 ATOM 775 OD2 <NA> ASP A 104 <NA> -6.568 -26.002 -9.460  
## 776 ATOM 776 N <NA> TYR A 105 <NA> -2.969 -23.881 -12.112  
## 777 ATOM 777 CA <NA> TYR A 105 <NA> -2.364 -23.232 -13.265  
## 778 ATOM 778 C <NA> TYR A 105 <NA> -1.754 -21.901 -13.021  
## 779 ATOM 779 O <NA> TYR A 105 <NA> -2.283 -21.077 -12.308  
## 780 ATOM 780 CB <NA> TYR A 105 <NA> -3.374 -23.004 -14.358  
## 781 ATOM 781 CG <NA> TYR A 105 <NA> -3.932 -24.246 -14.907  
## 782 ATOM 782 CD1 <NA> TYR A 105 <NA> -5.070 -24.809 -14.333  
## 783 ATOM 783 CD2 <NA> TYR A 105 <NA> -3.347 -24.877 -16.002  
## 784 ATOM 784 CE1 <NA> TYR A 105 <NA> -5.624 -25.978 -14.826  
## 785 ATOM 785 CE2 <NA> TYR A 105 <NA> -3.896 -26.061 -16.515  
## 786 ATOM 786 CZ <NA> TYR A 105 <NA> -5.041 -26.598 -15.909  
## 787 ATOM 787 OH <NA> TYR A 105 <NA> -5.623 -27.759 -16.356  
## 788 ATOM 788 N <NA> VAL A 106 <NA> -0.694 -21.659 -13.763  
## 789 ATOM 789 CA <NA> VAL A 106 <NA> 0.038 -20.419 -13.718  
## 790 ATOM 790 C <NA> VAL A 106 <NA> 0.133 -20.080 -15.186  
## 791 ATOM 791 O <NA> VAL A 106 <NA> 0.763 -20.799 -15.979  
## 792 ATOM 792 CB <NA> VAL A 106 <NA> 1.436 -20.615 -13.159  
## 793 ATOM 793 CG1 <NA> VAL A 106 <NA> 2.163 -19.304 -13.179  
## 794 ATOM 794 CG2 <NA> VAL A 106 <NA> 1.362 -21.183 -11.754  
## 795 ATOM 795 N <NA> LEU A 107 <NA> -0.591 -19.041 -15.559  
## 796 ATOM 796 CA <NA> LEU A 107 <NA> -0.631 -18.614 -16.936  
## 797 ATOM 797 C <NA> LEU A 107 <NA> 0.114 -17.314 -17.072  
## 798 ATOM 798 O <NA> LEU A 107 <NA> -0.049 -16.424 -16.259  
## 799 ATOM 799 CB <NA> LEU A 107 <NA> -2.079 -18.414 -17.370  
## 800 ATOM 800 CG <NA> LEU A 107 <NA> -3.071 -19.535 -17.051  
## 801 ATOM 801 CD1 <NA> LEU A 107 <NA> -4.463 -19.069 -17.428  
## 802 ATOM 802 CD2 <NA> LEU A 107 <NA> -2.724 -20.799 -17.807  
## 803 ATOM 803 N <NA> GLU A 108 <NA> 0.979 -17.227 -18.069  
## 804 ATOM 804 CA <NA> GLU A 108 <NA> 1.720 -16.011 -18.301  
## 805 ATOM 805 C <NA> GLU A 108 <NA> 1.173 -15.440 -19.582  
## 806 ATOM 806 O <NA> GLU A 108 <NA> 1.270 -16.058 -20.626  
## 807 ATOM 807 CB <NA> GLU A 108 <NA> 3.209 -16.288 -18.472  
## 808 ATOM 808 CG <NA> GLU A 108 <NA> 4.021 -14.992 -18.546  
## 809 ATOM 809 CD <NA> GLU A 108 <NA> 5.425 -15.174 -19.060  
## 810 ATOM 810 OE1 <NA> GLU A 108 <NA> 5.861 -16.335 -19.245  
## 811 ATOM 811 OE2 <NA> GLU A 108 <NA> 6.082 -14.131 -19.290  
## 812 ATOM 812 N <NA> PHE A 109 <NA> 0.566 -14.273 -19.489  
## 813 ATOM 813 CA <NA> PHE A 109 <NA> -0.008 -13.621 -20.634  
## 814 ATOM 814 C <NA> PHE A 109 <NA> 1.117 -12.841 -21.283  
## 815 ATOM 815 O <NA> PHE A 109 <NA> 1.519 -11.794 -20.802  
## 816 ATOM 816 CB <NA> PHE A 109 <NA> -1.113 -12.712 -20.156  
## 817 ATOM 817 CG <NA> PHE A 109 <NA> -2.099 -12.358 -21.208  
## 818 ATOM 818 CD1 <NA> PHE A 109 <NA> -3.182 -13.183 -21.451  
## 819 ATOM 819 CD2 <NA> PHE A 109 <NA> -2.016 -11.127 -21.873  
## 820 ATOM 820 CE1 <NA> PHE A 109 <NA> -4.186 -12.790 -22.330  
## 821 ATOM 821 CE2 <NA> PHE A 109 <NA> -3.020 -10.713 -22.763  
## 822 ATOM 822 CZ <NA> PHE A 109 <NA> -4.107 -11.546 -22.987  
## 823 ATOM 823 N <NA> ASP A 110 <NA> 1.596 -13.334 -22.412  
## 824 ATOM 824 CA <NA> ASP A 110 <NA> 2.733 -12.724 -23.092  
## 825 ATOM 825 C <NA> ASP A 110 <NA> 2.493 -11.719 -24.225  
## 826 ATOM 826 O <NA> ASP A 110 <NA> 1.869 -12.055 -25.224  
## 827 ATOM 827 CB <NA> ASP A 110 <NA> 3.603 -13.856 -23.615  
## 828 ATOM 828 CG <NA> ASP A 110 <NA> 4.915 -13.381 -24.131  
## 829 ATOM 829 OD1 <NA> ASP A 110 <NA> 5.602 -12.653 -23.394  
## 830 ATOM 830 OD2 <NA> ASP A 110 <NA> 5.255 -13.743 -25.276  
## 831 ATOM 831 N <NA> VAL A 111 <NA> 2.979 -10.490 -24.060  
## 832 ATOM 832 CA <NA> VAL A 111 <NA> 2.887 -9.442 -25.089  
## 833 ATOM 833 C <NA> VAL A 111 <NA> 4.222 -8.701 -25.064  
## 834 ATOM 834 O <NA> VAL A 111 <NA> 4.597 -8.130 -24.037  
## 835 ATOM 835 CB <NA> VAL A 111 <NA> 1.783 -8.417 -24.832  
## 836 ATOM 836 CG1 <NA> VAL A 111 <NA> 1.838 -7.346 -25.912  
## 837 ATOM 837 CG2 <NA> VAL A 111 <NA> 0.422 -9.095 -24.811  
## 838 ATOM 838 N <NA> PRO A 112 <NA> 4.967 -8.735 -26.181  
## 839 ATOM 839 CA <NA> PRO A 112 <NA> 6.278 -8.108 -26.392  
## 840 ATOM 840 C <NA> PRO A 112 <NA> 6.342 -6.667 -25.949  
## 841 ATOM 841 O <NA> PRO A 112 <NA> 5.510 -5.839 -26.328  
## 842 ATOM 842 CB <NA> PRO A 112 <NA> 6.471 -8.229 -27.900  
## 843 ATOM 843 CG <NA> PRO A 112 <NA> 5.791 -9.541 -28.202  
## 844 ATOM 844 CD <NA> PRO A 112 <NA> 4.516 -9.418 -27.408  
## 845 ATOM 845 N <NA> ASP A 113 <NA> 7.380 -6.361 -25.189  
## 846 ATOM 846 CA <NA> ASP A 113 <NA> 7.570 -5.021 -24.664  
## 847 ATOM 847 C <NA> ASP A 113 <NA> 7.311 -3.927 -25.661  
## 848 ATOM 848 O <NA> ASP A 113 <NA> 6.638 -2.954 -25.346  
## 849 ATOM 849 CB <NA> ASP A 113 <NA> 8.981 -4.846 -24.090  
## 850 ATOM 850 CG <NA> ASP A 113 <NA> 9.156 -5.514 -22.739  
## 851 ATOM 851 OD1 <NA> ASP A 113 <NA> 8.183 -6.118 -22.218  
## 852 ATOM 852 OD2 <NA> ASP A 113 <NA> 10.276 -5.411 -22.196  
## 853 ATOM 853 N <NA> GLU A 114 <NA> 7.874 -4.067 -26.854  
## 854 ATOM 854 CA <NA> GLU A 114 <NA> 7.702 -3.047 -27.883  
## 855 ATOM 855 C <NA> GLU A 114 <NA> 6.254 -2.841 -28.231  
## 856 ATOM 856 O <NA> GLU A 114 <NA> 5.824 -1.717 -28.432  
## 857 ATOM 857 CB <NA> GLU A 114 <NA> 8.491 -3.383 -29.155  
## 858 ATOM 858 CG <NA> GLU A 114 <NA> 9.983 -3.087 -29.072  
## 859 ATOM 859 CD <NA> GLU A 114 <NA> 10.278 -1.698 -28.530  
## 860 ATOM 860 OE1 <NA> GLU A 114 <NA> 9.791 -0.691 -29.115  
## 861 ATOM 861 OE2 <NA> GLU A 114 <NA> 10.999 -1.629 -27.506  
## 862 ATOM 862 N <NA> LEU A 115 <NA> 5.496 -3.927 -28.286  
## 863 ATOM 863 CA <NA> LEU A 115 <NA> 4.102 -3.807 -28.622  
## 864 ATOM 864 C <NA> LEU A 115 <NA> 3.358 -3.107 -27.513  
## 865 ATOM 865 O <NA> LEU A 115 <NA> 2.516 -2.251 -27.779  
## 866 ATOM 866 CB <NA> LEU A 115 <NA> 3.511 -5.164 -28.966  
## 867 ATOM 867 CG <NA> LEU A 115 <NA> 3.803 -5.594 -30.413  
## 868 ATOM 868 CD1 <NA> LEU A 115 <NA> 5.245 -6.019 -30.624  
## 869 ATOM 869 CD2 <NA> LEU A 115 <NA> 2.878 -6.720 -30.763  
## 870 ATOM 870 N <NA> ILE A 116 <NA> 3.728 -3.409 -26.267  
## 871 ATOM 871 CA <NA> ILE A 116 <NA> 3.103 -2.760 -25.109  
## 872 ATOM 872 C <NA> ILE A 116 <NA> 3.470 -1.267 -25.126  
## 873 ATOM 873 O <NA> ILE A 116 <NA> 2.614 -0.415 -24.873  
## 874 ATOM 874 CB <NA> ILE A 116 <NA> 3.588 -3.359 -23.749  
## 875 ATOM 875 CG1 <NA> ILE A 116 <NA> 3.043 -4.764 -23.535  
## 876 ATOM 876 CG2 <NA> ILE A 116 <NA> 3.142 -2.474 -22.595  
## 877 ATOM 877 CD1 <NA> ILE A 116 <NA> 3.656 -5.447 -22.326  
## 878 ATOM 878 N <NA> VAL A 117 <NA> 4.749 -0.965 -25.368  
## 879 ATOM 879 CA <NA> VAL A 117 <NA> 5.245 0.415 -25.424  
## 880 ATOM 880 C <NA> VAL A 117 <NA> 4.421 1.195 -26.442  
## 881 ATOM 881 O <NA> VAL A 117 <NA> 3.957 2.288 -26.146  
## 882 ATOM 882 CB <NA> VAL A 117 <NA> 6.727 0.499 -25.869  
## 883 ATOM 883 CG1 <NA> VAL A 117 <NA> 7.159 1.924 -25.890  
## 884 ATOM 884 CG2 <NA> VAL A 117 <NA> 7.626 -0.269 -24.949  
## 885 ATOM 885 N <NA> ASP A 118 <NA> 4.209 0.600 -27.617  
## 886 ATOM 886 CA <NA> ASP A 118 <NA> 3.433 1.204 -28.704  
## 887 ATOM 887 C <NA> ASP A 118 <NA> 1.970 1.386 -28.331  
## 888 ATOM 888 O <NA> ASP A 118 <NA> 1.332 2.373 -28.722  
## 889 ATOM 889 CB <NA> ASP A 118 <NA> 3.514 0.345 -29.971  
## 890 ATOM 890 CG <NA> ASP A 118 <NA> 4.943 0.221 -30.524  
## 891 ATOM 891 OD1 <NA> ASP A 118 <NA> 5.836 1.012 -30.129  
## 892 ATOM 892 OD2 <NA> ASP A 118 <NA> 5.176 -0.685 -31.360  
## 893 ATOM 893 N <NA> ARG A 119 <NA> 1.432 0.417 -27.601  
## 894 ATOM 894 CA <NA> ARG A 119 <NA> 0.045 0.469 -27.172  
## 895 ATOM 895 C <NA> ARG A 119 <NA> -0.177 1.561 -26.158  
## 896 ATOM 896 O <NA> ARG A 119 <NA> -1.291 2.021 -25.996  
## 897 ATOM 897 CB <NA> ARG A 119 <NA> -0.402 -0.871 -26.581  
## 898 ATOM 898 CG <NA> ARG A 119 <NA> -0.466 -1.996 -27.607  
## 899 ATOM 899 CD <NA> ARG A 119 <NA> -0.728 -3.357 -26.986  
## 900 ATOM 900 NE <NA> ARG A 119 <NA> -0.775 -4.407 -28.009  
## 901 ATOM 901 CZ <NA> ARG A 119 <NA> -1.142 -5.667 -27.779  
## 902 ATOM 902 NH1 <NA> ARG A 119 <NA> -1.483 -6.048 -26.555  
## 903 ATOM 903 NH2 <NA> ARG A 119 <NA> -1.159 -6.553 -28.768  
## 904 ATOM 904 N <NA> ILE A 120 <NA> 0.887 2.045 -25.538  
## 905 ATOM 905 CA <NA> ILE A 120 <NA> 0.711 3.053 -24.516  
## 906 ATOM 906 C <NA> ILE A 120 <NA> 1.254 4.431 -24.787  
## 907 ATOM 907 O <NA> ILE A 120 <NA> 0.517 5.400 -24.674  
## 908 ATOM 908 CB <NA> ILE A 120 <NA> 1.236 2.547 -23.145  
## 909 ATOM 909 CG1 <NA> ILE A 120 <NA> 0.346 1.416 -22.638  
## 910 ATOM 910 CG2 <NA> ILE A 120 <NA> 1.276 3.673 -22.121  
## 911 ATOM 911 CD1 <NA> ILE A 120 <NA> 1.037 0.511 -21.647  
## 912 ATOM 912 N <NA> VAL A 121 <NA> 2.528 4.551 -25.133  
## 913 ATOM 913 CA <NA> VAL A 121 <NA> 3.078 5.887 -25.342  
## 914 ATOM 914 C <NA> VAL A 121 <NA> 2.273 6.717 -26.340  
## 915 ATOM 915 O <NA> VAL A 121 <NA> 2.068 7.923 -26.134  
## 916 ATOM 916 CB <NA> VAL A 121 <NA> 4.584 5.868 -25.722  
## 917 ATOM 917 CG1 <NA> VAL A 121 <NA> 5.349 4.958 -24.784  
## 918 ATOM 918 CG2 <NA> VAL A 121 <NA> 4.781 5.470 -27.167  
## 919 ATOM 919 N <NA> GLY A 122 <NA> 1.727 6.045 -27.355  
## 920 ATOM 920 CA <NA> GLY A 122 <NA> 0.963 6.738 -28.375  
## 921 ATOM 921 C <NA> GLY A 122 <NA> -0.485 7.032 -28.044  
## 922 ATOM 922 O <NA> GLY A 122 <NA> -1.349 6.906 -28.917  
## 923 ATOM 923 N <NA> ARG A 123 <NA> -0.785 7.399 -26.803  
## 924 ATOM 924 CA <NA> ARG A 123 <NA> -2.167 7.692 -26.465  
## 925 ATOM 925 C <NA> ARG A 123 <NA> -2.349 9.062 -25.856  
## 926 ATOM 926 O <NA> ARG A 123 <NA> -1.581 9.486 -24.985  
## 927 ATOM 927 CB <NA> ARG A 123 <NA> -2.818 6.581 -25.616  
## 928 ATOM 928 CG <NA> ARG A 123 <NA> -2.507 6.553 -24.137  
## 929 ATOM 929 CD <NA> ARG A 123 <NA> -3.358 5.488 -23.448  
## 930 ATOM 930 NE <NA> ARG A 123 <NA> -2.966 5.312 -22.058  
## 931 ATOM 931 CZ <NA> ARG A 123 <NA> -2.623 4.145 -21.522  
## 932 ATOM 932 NH1 <NA> ARG A 123 <NA> -2.660 3.036 -22.248  
## 933 ATOM 933 NH2 <NA> ARG A 123 <NA> -2.262 4.081 -20.248  
## 934 ATOM 934 N <NA> ARG A 124 <NA> -3.333 9.767 -26.416  
## 935 ATOM 935 CA <NA> ARG A 124 <NA> -3.720 11.125 -26.034  
## 936 ATOM 936 C <NA> ARG A 124 <NA> -5.060 11.016 -25.300  
## 937 ATOM 937 O <NA> ARG A 124 <NA> -5.944 10.262 -25.718  
## 938 ATOM 938 CB <NA> ARG A 124 <NA> -3.900 11.999 -27.286  
## 939 ATOM 939 CG <NA> ARG A 124 <NA> -2.811 11.864 -28.356  
## 940 ATOM 940 CD <NA> ARG A 124 <NA> -1.474 12.515 -27.972  
## 941 ATOM 941 NE <NA> ARG A 124 <NA> -0.534 12.491 -29.098  
## 942 ATOM 942 CZ <NA> ARG A 124 <NA> 0.496 11.652 -29.205  
## 943 ATOM 943 NH1 <NA> ARG A 124 <NA> 0.753 10.780 -28.236  
## 944 ATOM 944 NH2 <NA> ARG A 124 <NA> 1.286 11.701 -30.273  
## 945 ATOM 945 N <NA> VAL A 125 <NA> -5.232 11.816 -24.257  
## 946 ATOM 946 CA <NA> VAL A 125 <NA> -6.439 11.778 -23.450  
## 947 ATOM 947 C <NA> VAL A 125 <NA> -7.066 13.153 -23.227  
## 948 ATOM 948 O <NA> VAL A 125 <NA> -6.369 14.167 -23.167  
## 949 ATOM 949 CB <NA> VAL A 125 <NA> -6.127 11.154 -22.049  
## 950 ATOM 950 CG1 <NA> VAL A 125 <NA> -5.422 9.809 -22.206  
## 951 ATOM 951 CG2 <NA> VAL A 125 <NA> -5.255 12.093 -21.214  
## 952 ATOM 952 N <NA> HIS A 126 <NA> -8.388 13.205 -23.159  
## 953 ATOM 953 CA <NA> HIS A 126 <NA> -9.028 14.474 -22.864  
## 954 ATOM 954 C <NA> HIS A 126 <NA> -9.128 14.522 -21.346  
## 955 ATOM 955 O <NA> HIS A 126 <NA> -10.022 13.905 -20.756  
## 956 ATOM 956 CB <NA> HIS A 126 <NA> -10.424 14.602 -23.466  
## 957 ATOM 957 CG <NA> HIS A 126 <NA> -11.085 15.901 -23.122  
## 958 ATOM 958 ND1 <NA> HIS A 126 <NA> -10.399 17.097 -23.110  
## 959 ATOM 959 CD2 <NA> HIS A 126 <NA> -12.338 16.183 -22.694  
## 960 ATOM 960 CE1 <NA> HIS A 126 <NA> -11.198 18.057 -22.679  
## 961 ATOM 961 NE2 <NA> HIS A 126 <NA> -12.380 17.529 -22.421  
## 962 ATOM 962 N <NA> ALA A 127 <NA> -8.212 15.261 -20.728  
## 963 ATOM 963 CA <NA> ALA A 127 <NA> -8.159 15.378 -19.275  
## 964 ATOM 964 C <NA> ALA A 127 <NA> -9.507 15.494 -18.525  
## 965 ATOM 965 O <NA> ALA A 127 <NA> -9.860 14.582 -17.767  
## 966 ATOM 966 CB <NA> ALA A 127 <NA> -7.180 16.486 -18.863  
## 967 ATOM 967 N <NA> PRO A 128 <NA> -10.279 16.596 -18.727  
## 968 ATOM 968 CA <NA> PRO A 128 <NA> -11.571 16.743 -18.026  
## 969 ATOM 969 C <NA> PRO A 128 <NA> -12.766 15.958 -18.619  
## 970 ATOM 970 O <NA> PRO A 128 <NA> -13.784 16.548 -19.003  
## 971 ATOM 971 CB <NA> PRO A 128 <NA> -11.828 18.266 -18.082  
## 972 ATOM 972 CG <NA> PRO A 128 <NA> -10.467 18.874 -18.375  
## 973 ATOM 973 CD <NA> PRO A 128 <NA> -9.903 17.877 -19.357  
## 974 ATOM 974 N <NA> SER A 129 <NA> -12.644 14.634 -18.672  
## 975 ATOM 975 CA <NA> SER A 129 <NA> -13.695 13.757 -19.199  
## 976 ATOM 976 C <NA> SER A 129 <NA> -13.192 12.322 -19.119  
## 977 ATOM 977 O <NA> SER A 129 <NA> -13.970 11.374 -18.959  
## 978 ATOM 978 CB <NA> SER A 129 <NA> -14.011 14.096 -20.656  
## 979 ATOM 979 OG <NA> SER A 129 <NA> -12.925 13.771 -21.517  
## 980 ATOM 980 N <NA> GLY A 130 <NA> -11.878 12.185 -19.285  
## 981 ATOM 981 CA <NA> GLY A 130 <NA> -11.241 10.889 -19.225  
## 982 ATOM 982 C <NA> GLY A 130 <NA> -11.185 10.173 -20.557  
## 983 ATOM 983 O <NA> GLY A 130 <NA> -10.603 9.090 -20.632  
## 984 ATOM 984 N <NA> ARG A 131 <NA> -11.774 10.759 -21.601  
## 985 ATOM 985 CA <NA> ARG A 131 <NA> -11.770 10.135 -22.926  
## 986 ATOM 986 C <NA> ARG A 131 <NA> -10.342 9.841 -23.385  
## 987 ATOM 987 O <NA> ARG A 131 <NA> -9.442 10.669 -23.203  
## 988 ATOM 988 CB <NA> ARG A 131 <NA> -12.491 11.014 -23.946  
## 989 ATOM 989 CG <NA> ARG A 131 <NA> -13.945 10.619 -24.193  
## 990 ATOM 990 CD <NA> ARG A 131 <NA> -14.923 11.593 -23.556  
## 991 ATOM 991 NE <NA> ARG A 131 <NA> -14.716 12.969 -24.006  
## 992 ATOM 992 CZ <NA> ARG A 131 <NA> -15.408 14.007 -23.552  
## 993 ATOM 993 NH1 <NA> ARG A 131 <NA> -16.351 13.835 -22.635  
## 994 ATOM 994 NH2 <NA> ARG A 131 <NA> -15.154 15.222 -24.004  
## 995 ATOM 995 N <NA> VAL A 132 <NA> -10.145 8.673 -23.995  
## 996 ATOM 996 CA <NA> VAL A 132 <NA> -8.814 8.251 -24.434  
## 997 ATOM 997 C <NA> VAL A 132 <NA> -8.738 7.874 -25.911  
## 998 ATOM 998 O <NA> VAL A 132 <NA> -9.602 7.166 -26.442  
## 999 ATOM 999 CB <NA> VAL A 132 <NA> -8.275 7.077 -23.548  
## 1000 ATOM 1000 CG1 <NA> VAL A 132 <NA> -9.055 5.801 -23.814  
## 1001 ATOM 1001 CG2 <NA> VAL A 132 <NA> -6.796 6.860 -23.781  
## 1002 ATOM 1002 N <NA> TYR A 133 <NA> -7.678 8.344 -26.555  
## 1003 ATOM 1003 CA <NA> TYR A 133 <NA> -7.447 8.105 -27.966  
## 1004 ATOM 1004 C <NA> TYR A 133 <NA> -6.090 7.485 -28.117  
## 1005 ATOM 1005 O <NA> TYR A 133 <NA> -5.314 7.447 -27.164  
## 1006 ATOM 1006 CB <NA> TYR A 133 <NA> -7.451 9.437 -28.726  
## 1007 ATOM 1007 CG <NA> TYR A 133 <NA> -8.713 10.218 -28.511  
## 1008 ATOM 1008 CD1 <NA> TYR A 133 <NA> -9.834 10.002 -29.313  
## 1009 ATOM 1009 CD2 <NA> TYR A 133 <NA> -8.823 11.106 -27.445  
## 1010 ATOM 1010 CE1 <NA> TYR A 133 <NA> -11.035 10.641 -29.050  
## 1011 ATOM 1011 CE2 <NA> TYR A 133 <NA> -10.020 11.754 -27.170  
## 1012 ATOM 1012 CZ <NA> TYR A 133 <NA> -11.122 11.516 -27.973  
## 1013 ATOM 1013 OH <NA> TYR A 133 <NA> -12.316 12.143 -27.681  
## 1014 ATOM 1014 N <NA> HIS A 134 <NA> -5.839 6.950 -29.305  
## 1015 ATOM 1015 CA <NA> HIS A 134 <NA> -4.543 6.390 -29.661  
## 1016 ATOM 1016 C <NA> HIS A 134 <NA> -4.231 6.776 -31.115  
## 1017 ATOM 1017 O <NA> HIS A 134 <NA> -4.827 6.234 -32.049  
## 1018 ATOM 1018 CB <NA> HIS A 134 <NA> -4.474 4.871 -29.497  
## 1019 ATOM 1019 CG <NA> HIS A 134 <NA> -3.086 4.333 -29.676  
## 1020 ATOM 1020 ND1 <NA> HIS A 134 <NA> -2.531 4.095 -30.911  
## 1021 ATOM 1021 CD2 <NA> HIS A 134 <NA> -2.116 4.060 -28.770  
## 1022 ATOM 1022 CE1 <NA> HIS A 134 <NA> -1.281 3.697 -30.765  
## 1023 ATOM 1023 NE2 <NA> HIS A 134 <NA> -1.002 3.667 -29.476  
## 1024 ATOM 1024 N <NA> VAL A 135 <NA> -3.272 7.685 -31.284  
## 1025 ATOM 1025 CA <NA> VAL A 135 <NA> -2.851 8.189 -32.585  
## 1026 ATOM 1026 C <NA> VAL A 135 <NA> -2.996 7.184 -33.721  
## 1027 ATOM 1027 O <NA> VAL A 135 <NA> -3.278 7.567 -34.853  
## 1028 ATOM 1028 CB <NA> VAL A 135 <NA> -1.408 8.723 -32.548  
## 1029 ATOM 1029 CG1 <NA> VAL A 135 <NA> -1.332 9.958 -31.659  
## 1030 ATOM 1030 CG2 <NA> VAL A 135 <NA> -0.450 7.652 -32.057  
## 1031 ATOM 1031 N <NA> LYS A 136 <NA> -2.780 5.904 -33.431  
## 1032 ATOM 1032 CA <NA> LYS A 136 <NA> -2.947 4.882 -34.453  
## 1033 ATOM 1033 C <NA> LYS A 136 <NA> -4.286 4.175 -34.306  
## 1034 ATOM 1034 O <NA> LYS A 136 <NA> -5.138 4.279 -35.180  
## 1035 ATOM 1035 CB <NA> LYS A 136 <NA> -1.819 3.841 -34.415  
## 1036 ATOM 1036 CG <NA> LYS A 136 <NA> -0.456 4.320 -34.899  
## 1037 ATOM 1037 CD <NA> LYS A 136 <NA> 0.394 4.850 -33.739  
## 1038 ATOM 1038 CE <NA> LYS A 136 <NA> 1.769 5.375 -34.187  
## 1039 ATOM 1039 NZ <NA> LYS A 136 <NA> 2.563 5.925 -33.036  
## 1040 ATOM 1040 N <NA> PHE A 137 <NA> -4.489 3.535 -33.154  
## 1041 ATOM 1041 CA <NA> PHE A 137 <NA> -5.691 2.739 -32.873  
## 1042 ATOM 1042 C <NA> PHE A 137 <NA> -7.058 3.406 -32.864  
## 1043 ATOM 1043 O <NA> PHE A 137 <NA> -8.012 2.839 -33.395  
## 1044 ATOM 1044 CB <NA> PHE A 137 <NA> -5.481 1.891 -31.611  
## 1045 ATOM 1045 CG <NA> PHE A 137 <NA> -4.126 1.228 -31.557  
## 1046 ATOM 1046 CD1 <NA> PHE A 137 <NA> -3.505 0.785 -32.722  
## 1047 ATOM 1047 CD2 <NA> PHE A 137 <NA> -3.428 1.143 -30.360  
## 1048 ATOM 1048 CE1 <NA> PHE A 137 <NA> -2.213 0.285 -32.700  
## 1049 ATOM 1049 CE2 <NA> PHE A 137 <NA> -2.128 0.640 -30.327  
## 1050 ATOM 1050 CZ <NA> PHE A 137 <NA> -1.519 0.214 -31.500  
## 1051 ATOM 1051 N <NA> ASN A 138 <NA> -7.182 4.560 -32.215  
## 1052 ATOM 1052 CA <NA> ASN A 138 <NA> -8.460 5.283 -32.185  
## 1053 ATOM 1053 C <NA> ASN A 138 <NA> -8.200 6.783 -32.173  
## 1054 ATOM 1054 O <NA> ASN A 138 <NA> -8.435 7.476 -31.183  
## 1055 ATOM 1055 CB <NA> ASN A 138 <NA> -9.377 4.838 -31.017  
## 1056 ATOM 1056 CG <NA> ASN A 138 <NA> -8.969 5.414 -29.658  
## 1057 ATOM 1057 OD1 <NA> ASN A 138 <NA> -7.824 5.268 -29.218  
## 1058 ATOM 1058 ND2 <NA> ASN A 138 <NA> -9.916 6.064 -28.988  
## 1059 ATOM 1059 N <NA> PRO A 139 <NA> -7.686 7.302 -33.290  
## 1060 ATOM 1060 CA <NA> PRO A 139 <NA> -7.389 8.735 -33.401  
## 1061 ATOM 1061 C <NA> PRO A 139 <NA> -8.636 9.594 -33.286  
## 1062 ATOM 1062 O <NA> PRO A 139 <NA> -9.752 9.120 -33.508  
## 1063 ATOM 1063 CB <NA> PRO A 139 <NA> -6.777 8.842 -34.796  
## 1064 ATOM 1064 CG <NA> PRO A 139 <NA> -7.479 7.737 -35.565  
## 1065 ATOM 1065 CD <NA> PRO A 139 <NA> -7.448 6.604 -34.570  
## 1066 ATOM 1066 N <NA> PRO A 140 <NA> -8.482 10.835 -32.815  
## 1067 ATOM 1067 CA <NA> PRO A 140 <NA> -9.686 11.650 -32.732  
## 1068 ATOM 1068 C <NA> PRO A 140 <NA> -9.997 12.139 -34.146  
## 1069 ATOM 1069 O <NA> PRO A 140 <NA> -9.114 12.147 -35.011  
## 1070 ATOM 1070 CB <NA> PRO A 140 <NA> -9.262 12.784 -31.800  
## 1071 ATOM 1071 CG <NA> PRO A 140 <NA> -7.821 12.918 -32.060  
## 1072 ATOM 1072 CD <NA> PRO A 140 <NA> -7.352 11.488 -32.142  
## 1073 ATOM 1073 N <NA> LYS A 141 <NA> -11.262 12.472 -34.399  
## 1074 ATOM 1074 CA <NA> LYS A 141 <NA> -11.703 12.964 -35.707  
## 1075 ATOM 1075 C <NA> LYS A 141 <NA> -10.806 14.130 -36.090  
## 1076 ATOM 1076 O <NA> LYS A 141 <NA> -10.231 14.159 -37.175  
## 1077 ATOM 1077 CB <NA> LYS A 141 <NA> -13.167 13.419 -35.650  
## 1078 ATOM 1078 CG <NA> LYS A 141 <NA> -14.184 12.303 -35.414  
## 1079 ATOM 1079 CD <NA> LYS A 141 <NA> -15.564 12.893 -35.191  
## 1080 ATOM 1080 CE <NA> LYS A 141 <NA> -16.506 11.889 -34.550  
## 1081 ATOM 1081 NZ <NA> LYS A 141 <NA> -17.664 12.574 -33.885  
## 1082 ATOM 1082 N <NA> VAL A 142 <NA> -10.726 15.110 -35.202  
## 1083 ATOM 1083 CA <NA> VAL A 142 <NA> -9.854 16.249 -35.428  
## 1084 ATOM 1084 C <NA> VAL A 142 <NA> -8.649 15.832 -34.602  
## 1085 ATOM 1085 O <NA> VAL A 142 <NA> -8.681 15.895 -33.366  
## 1086 ATOM 1086 CB <NA> VAL A 142 <NA> -10.444 17.559 -34.864  
## 1087 ATOM 1087 CG1 <NA> VAL A 142 <NA> -9.603 18.746 -35.315  
## 1088 ATOM 1088 CG2 <NA> VAL A 142 <NA> -11.891 17.722 -35.304  
## 1089 ATOM 1089 N <NA> GLU A 143 <NA> -7.644 15.288 -35.279  
## 1090 ATOM 1090 CA <NA> GLU A 143 <NA> -6.442 14.821 -34.608  
## 1091 ATOM 1091 C <NA> GLU A 143 <NA> -5.853 15.885 -33.671  
## 1092 ATOM 1092 O <NA> GLU A 143 <NA> -5.673 17.045 -34.060  
## 1093 ATOM 1093 CB <NA> GLU A 143 <NA> -5.416 14.328 -35.634  
## 1094 ATOM 1094 CG <NA> GLU A 143 <NA> -4.122 13.746 -35.038  
## 1095 ATOM 1095 CD <NA> GLU A 143 <NA> -4.235 12.312 -34.514  
## 1096 ATOM 1096 OE1 <NA> GLU A 143 <NA> -4.635 11.406 -35.287  
## 1097 ATOM 1097 OE2 <NA> GLU A 143 <NA> -3.869 12.094 -33.333  
## 1098 ATOM 1098 N <NA> GLY A 144 <NA> -5.607 15.473 -32.423  
## 1099 ATOM 1099 CA <NA> GLY A 144 <NA> -5.069 16.360 -31.402  
## 1100 ATOM 1100 C <NA> GLY A 144 <NA> -6.166 17.117 -30.671  
## 1101 ATOM 1101 O <NA> GLY A 144 <NA> -5.901 17.828 -29.699  
## 1102 ATOM 1102 N <NA> LYS A 145 <NA> -7.410 16.904 -31.095  
## 1103 ATOM 1103 CA <NA> LYS A 145 <NA> -8.567 17.580 -30.522  
## 1104 ATOM 1104 C <NA> LYS A 145 <NA> -9.608 16.576 -30.057  
## 1105 ATOM 1105 O <NA> LYS A 145 <NA> -9.902 15.601 -30.760  
## 1106 ATOM 1106 CB <NA> LYS A 145 <NA> -9.214 18.463 -31.592  
## 1107 ATOM 1107 CG <NA> LYS A 145 <NA> -8.310 19.494 -32.221  
## 1108 ATOM 1108 CD <NA> LYS A 145 <NA> -8.319 20.766 -31.424  
## 1109 ATOM 1109 CE <NA> LYS A 145 <NA> -7.701 21.899 -32.218  
## 1110 ATOM 1110 NZ <NA> LYS A 145 <NA> -7.916 23.232 -31.575  
## 1111 ATOM 1111 N <NA> ASP A 146 <NA> -10.194 16.838 -28.895  
## 1112 ATOM 1112 CA <NA> ASP A 146 <NA> -11.239 15.970 -28.344  
## 1113 ATOM 1113 C <NA> ASP A 146 <NA> -12.524 16.157 -29.148  
## 1114 ATOM 1114 O <NA> ASP A 146 <NA> -13.059 17.270 -29.250  
## 1115 ATOM 1115 CB <NA> ASP A 146 <NA> -11.481 16.269 -26.856  
## 1116 ATOM 1116 CG <NA> ASP A 146 <NA> -12.724 15.589 -26.316  
## 1117 ATOM 1117 OD1 <NA> ASP A 146 <NA> -12.882 14.359 -26.481  
## 1118 ATOM 1118 OD2 <NA> ASP A 146 <NA> -13.559 16.306 -25.732  
## 1119 ATOM 1119 N <NA> ASP A 147 <NA> -13.040 15.045 -29.658  
## 1120 ATOM 1120 CA <NA> ASP A 147 <NA> -14.240 15.020 -30.488  
## 1121 ATOM 1121 C <NA> ASP A 147 <NA> -15.532 15.569 -29.907  
## 1122 ATOM 1122 O <NA> ASP A 147 <NA> -16.393 16.040 -30.651  
## 1123 ATOM 1123 CB <NA> ASP A 147 <NA> -14.476 13.600 -30.987  
## 1124 ATOM 1124 CG <NA> ASP A 147 <NA> -13.333 13.093 -31.828  
## 1125 ATOM 1125 OD1 <NA> ASP A 147 <NA> -12.535 13.937 -32.319  
## 1126 ATOM 1126 OD2 <NA> ASP A 147 <NA> -13.241 11.853 -31.997  
## 1127 ATOM 1127 N <NA> VAL A 148 <NA> -15.682 15.487 -28.589  
## 1128 ATOM 1128 CA <NA> VAL A 148 <NA> -16.894 15.968 -27.932  
## 1129 ATOM 1129 C <NA> VAL A 148 <NA> -16.886 17.437 -27.503  
## 1130 ATOM 1130 O <NA> VAL A 148 <NA> -17.931 18.080 -27.500  
## 1131 ATOM 1131 CB <NA> VAL A 148 <NA> -17.278 15.031 -26.761  
## 1132 ATOM 1132 CG1 <NA> VAL A 148 <NA> -18.016 15.785 -25.652  
## 1133 ATOM 1133 CG2 <NA> VAL A 148 <NA> -18.137 13.895 -27.300  
## 1134 ATOM 1134 N <NA> THR A 149 <NA> -15.712 17.982 -27.203  
## 1135 ATOM 1135 CA <NA> THR A 149 <NA> -15.623 19.374 -26.767  
## 1136 ATOM 1136 C <NA> THR A 149 <NA> -14.811 20.278 -27.701  
## 1137 ATOM 1137 O <NA> THR A 149 <NA> -14.901 21.510 -27.626  
## 1138 ATOM 1138 CB <NA> THR A 149 <NA> -15.000 19.457 -25.376  
## 1139 ATOM 1139 OG1 <NA> THR A 149 <NA> -13.665 18.948 -25.437  
## 1140 ATOM 1140 CG2 <NA> THR A 149 <NA> -15.801 18.634 -24.384  
## 1141 ATOM 1141 N <NA> GLY A 150 <NA> -14.050 19.672 -28.606  
## 1142 ATOM 1142 CA <NA> GLY A 150 <NA> -13.222 20.470 -29.487  
## 1143 ATOM 1143 C <NA> GLY A 150 <NA> -12.180 21.096 -28.583  
## 1144 ATOM 1144 O <NA> GLY A 150 <NA> -11.793 22.256 -28.745  
## 1145 ATOM 1145 N <NA> GLU A 151 <NA> -11.765 20.314 -27.589  
## 1146 ATOM 1146 CA <NA> GLU A 151 <NA> -10.771 20.738 -26.611  
## 1147 ATOM 1147 C <NA> GLU A 151 <NA> -9.517 19.890 -26.810  
## 1148 ATOM 1148 O <NA> GLU A 151 <NA> -9.610 18.696 -27.093  
## 1149 ATOM 1149 CB <NA> GLU A 151 <NA> -11.327 20.553 -25.196  
## 1150 ATOM 1150 CG <NA> GLU A 151 <NA> -10.614 21.343 -24.100  
## 1151 ATOM 1151 CD <NA> GLU A 151 <NA> -11.304 21.226 -22.742  
## 1152 ATOM 1152 OE1 <NA> GLU A 151 <NA> -12.533 20.991 -22.707  
## 1153 ATOM 1153 OE2 <NA> GLU A 151 <NA> -10.616 21.362 -21.706  
## 1154 ATOM 1154 N <NA> GLU A 152 <NA> -8.349 20.504 -26.668  
## 1155 ATOM 1155 CA <NA> GLU A 152 <NA> -7.096 19.788 -26.860  
## 1156 ATOM 1156 C <NA> GLU A 152 <NA> -6.891 18.600 -25.926  
## 1157 ATOM 1157 O <NA> GLU A 152 <NA> -7.337 18.588 -24.770  
## 1158 ATOM 1158 CB <NA> GLU A 152 <NA> -5.902 20.743 -26.784  
## 1159 ATOM 1159 CG <NA> GLU A 152 <NA> -5.801 21.704 -27.972  
## 1160 ATOM 1160 CD <NA> GLU A 152 <NA> -4.757 21.297 -29.007  
## 1161 ATOM 1161 OE1 <NA> GLU A 152 <NA> -4.731 20.115 -29.418  
## 1162 ATOM 1162 OE2 <NA> GLU A 152 <NA> -3.965 22.177 -29.416  
## 1163 ATOM 1163 N <NA> LEU A 153 <NA> -6.240 17.584 -26.472  
## 1164 ATOM 1164 CA <NA> LEU A 153 <NA> -5.950 16.369 -25.742  
## 1165 ATOM 1165 C <NA> LEU A 153 <NA> -4.543 16.448 -25.172  
## 1166 ATOM 1166 O <NA> LEU A 153 <NA> -3.738 17.289 -25.586  
## 1167 ATOM 1167 CB <NA> LEU A 153 <NA> -6.064 15.169 -26.679  
## 1168 ATOM 1168 CG <NA> LEU A 153 <NA> -7.386 14.988 -27.419  
## 1169 ATOM 1169 CD1 <NA> LEU A 153 <NA> -7.268 13.807 -28.357  
## 1170 ATOM 1170 CD2 <NA> LEU A 153 <NA> -8.505 14.780 -26.427  
## 1171 ATOM 1171 N <NA> THR A 154 <NA> -4.235 15.526 -24.266  
## 1172 ATOM 1172 CA <NA> THR A 154 <NA> -2.938 15.471 -23.603  
## 1173 ATOM 1173 C <NA> THR A 154 <NA> -2.388 14.047 -23.503  
## 1174 ATOM 1174 O <NA> THR A 154 <NA> -2.965 13.100 -24.023  
## 1175 ATOM 1175 CB <NA> THR A 154 <NA> -3.065 16.032 -22.181  
## 1176 ATOM 1176 OG1 <NA> THR A 154 <NA> -4.289 15.558 -21.597  
## 1177 ATOM 1177 CG2 <NA> THR A 154 <NA> -3.070 17.550 -22.206  
## 1178 ATOM 1178 N <NA> THR A 155 <NA> -1.233 13.906 -22.881  
## 1179 ATOM 1179 CA <NA> THR A 155 <NA> -0.653 12.593 -22.699  
## 1180 ATOM 1180 C <NA> THR A 155 <NA> -0.515 12.445 -21.207  
## 1181 ATOM 1181 O <NA> THR A 155 <NA> -0.205 13.421 -20.521  
## 1182 ATOM 1182 CB <NA> THR A 155 <NA> 0.724 12.480 -23.352  
## 1183 ATOM 1183 OG1 <NA> THR A 155 <NA> 1.319 13.783 -23.447  
## 1184 ATOM 1184 CG2 <NA> THR A 155 <NA> 0.593 11.861 -24.730  
## 1185 ATOM 1185 N <NA> ARG A 156 <NA> -0.852 11.271 -20.692  
## 1186 ATOM 1186 CA <NA> ARG A 156 <NA> -0.733 11.036 -19.264  
## 1187 ATOM 1187 C <NA> ARG A 156 <NA> 0.770 10.912 -18.943  
## 1188 ATOM 1188 O <NA> ARG A 156 <NA> 1.577 10.587 -19.823  
## 1189 ATOM 1189 CB <NA> ARG A 156 <NA> -1.477 9.753 -18.886  
## 1190 ATOM 1190 CG <NA> ARG A 156 <NA> -2.244 9.818 -17.571  
## 1191 ATOM 1191 CD <NA> ARG A 156 <NA> -2.705 8.424 -17.089  
## 1192 ATOM 1192 NE <NA> ARG A 156 <NA> -3.553 7.709 -18.048  
## 1193 ATOM 1193 CZ <NA> ARG A 156 <NA> -4.870 7.878 -18.184  
## 1194 ATOM 1194 NH1 <NA> ARG A 156 <NA> -5.530 8.759 -17.440  
## 1195 ATOM 1195 NH2 <NA> ARG A 156 <NA> -5.533 7.167 -19.088  
## 1196 ATOM 1196 N <NA> LYS A 157 <NA> 1.151 11.196 -17.698  
## 1197 ATOM 1197 CA <NA> LYS A 157 <NA> 2.560 11.095 -17.291  
## 1198 ATOM 1198 C <NA> LYS A 157 <NA> 3.022 9.646 -17.408  
## 1199 ATOM 1199 O <NA> LYS A 157 <NA> 4.129 9.364 -17.868  
## 1200 ATOM 1200 CB <NA> LYS A 157 <NA> 2.747 11.587 -15.846  
## 1201 ATOM 1201 CG <NA> LYS A 157 <NA> 4.131 11.285 -15.234  
## 1202 ATOM 1202 CD <NA> LYS A 157 <NA> 5.283 11.938 -16.010  
## 1203 ATOM 1203 CE <NA> LYS A 157 <NA> 5.409 13.437 -15.727  
## 1204 ATOM 1204 NZ <NA> LYS A 157 <NA> 5.938 13.743 -14.360  
## 1205 ATOM 1205 N <NA> ASP A 158 <NA> 2.135 8.743 -17.007  
## 1206 ATOM 1206 CA <NA> ASP A 158 <NA> 2.384 7.312 -17.042  
## 1207 ATOM 1207 C <NA> ASP A 158 <NA> 2.666 6.839 -18.456  
## 1208 ATOM 1208 O <NA> ASP A 158 <NA> 3.540 6.005 -18.671  
## 1209 ATOM 1209 CB <NA> ASP A 158 <NA> 1.166 6.556 -16.501  
## 1210 ATOM 1210 CG <NA> ASP A 158 <NA> 0.770 6.994 -15.101  
## 1211 ATOM 1211 OD1 <NA> ASP A 158 <NA> 1.650 7.439 -14.330  
## 1212 ATOM 1212 OD2 <NA> ASP A 158 <NA> -0.433 6.886 -14.776  
## 1213 ATOM 1213 N <NA> ASP A 159 <NA> 1.926 7.390 -19.413  
## 1214 ATOM 1214 CA <NA> ASP A 159 <NA> 2.061 7.029 -20.815  
## 1215 ATOM 1215 C <NA> ASP A 159 <NA> 3.418 7.376 -21.411  
## 1216 ATOM 1216 O <NA> ASP A 159 <NA> 3.785 6.866 -22.464  
## 1217 ATOM 1217 CB <NA> ASP A 159 <NA> 0.956 7.696 -21.618  
## 1218 ATOM 1218 CG <NA> ASP A 159 <NA> -0.430 7.410 -21.060  
## 1219 ATOM 1219 OD1 <NA> ASP A 159 <NA> -0.545 6.562 -20.141  
## 1220 ATOM 1220 OD2 <NA> ASP A 159 <NA> -1.397 8.047 -21.550  
## 1221 ATOM 1221 N <NA> GLN A 160 <NA> 4.169 8.225 -20.721  
## 1222 ATOM 1222 CA <NA> GLN A 160 <NA> 5.498 8.640 -21.167  
## 1223 ATOM 1223 C <NA> GLN A 160 <NA> 6.410 7.457 -21.454  
## 1224 ATOM 1224 O <NA> GLN A 160 <NA> 6.620 6.609 -20.599  
## 1225 ATOM 1225 CB <NA> GLN A 160 <NA> 6.140 9.535 -20.111  
## 1226 ATOM 1226 CG <NA> GLN A 160 <NA> 6.023 11.016 -20.398  
## 1227 ATOM 1227 CD <NA> GLN A 160 <NA> 7.370 11.642 -20.734  
## 1228 ATOM 1228 OE1 <NA> GLN A 160 <NA> 8.332 10.948 -21.103  
## 1229 ATOM 1229 NE2 <NA> GLN A 160 <NA> 7.449 12.960 -20.601  
## 1230 ATOM 1230 N <NA> GLU A 161 <NA> 7.031 7.468 -22.622  
## 1231 ATOM 1231 CA <NA> GLU A 161 <NA> 7.901 6.382 -23.030  
## 1232 ATOM 1232 C <NA> GLU A 161 <NA> 8.967 5.994 -22.019  
## 1233 ATOM 1233 O <NA> GLU A 161 <NA> 9.193 4.806 -21.782  
## 1234 ATOM 1234 CB <NA> GLU A 161 <NA> 8.530 6.693 -24.382  
## 1235 ATOM 1235 CG <NA> GLU A 161 <NA> 8.932 5.445 -25.173  
## 1236 ATOM 1236 CD <NA> GLU A 161 <NA> 9.304 5.744 -26.624  
## 1237 ATOM 1237 OE1 <NA> GLU A 161 <NA> 8.419 6.173 -27.403  
## 1238 ATOM 1238 OE2 <NA> GLU A 161 <NA> 10.484 5.536 -26.988  
## 1239 ATOM 1239 N <NA> GLU A 162 <NA> 9.612 6.989 -21.418  
## 1240 ATOM 1240 CA <NA> GLU A 162 <NA> 10.659 6.758 -20.410  
## 1241 ATOM 1241 C <NA> GLU A 162 <NA> 10.104 6.027 -19.182  
## 1242 ATOM 1242 O <NA> GLU A 162 <NA> 10.739 5.128 -18.631  
## 1243 ATOM 1243 CB <NA> GLU A 162 <NA> 11.269 8.094 -19.971  
## 1244 ATOM 1244 CG <NA> GLU A 162 <NA> 12.210 8.006 -18.762  
## 1245 ATOM 1245 CD <NA> GLU A 162 <NA> 11.938 9.091 -17.718  
## 1246 ATOM 1246 OE1 <NA> GLU A 162 <NA> 11.062 8.874 -16.841  
## 1247 ATOM 1247 OE2 <NA> GLU A 162 <NA> 12.598 10.157 -17.783  
## 1248 ATOM 1248 N <NA> THR A 163 <NA> 8.924 6.446 -18.747  
## 1249 ATOM 1249 CA <NA> THR A 163 <NA> 8.260 5.844 -17.612  
## 1250 ATOM 1250 C <NA> THR A 163 <NA> 7.837 4.416 -17.961  
## 1251 ATOM 1251 O <NA> THR A 163 <NA> 8.109 3.485 -17.202  
## 1252 ATOM 1252 CB <NA> THR A 163 <NA> 7.045 6.688 -17.227  
## 1253 ATOM 1253 OG1 <NA> THR A 163 <NA> 7.485 8.028 -16.966  
## 1254 ATOM 1254 CG2 <NA> THR A 163 <NA> 6.362 6.138 -15.994  
## 1255 ATOM 1255 N <NA> VAL A 164 <NA> 7.248 4.229 -19.142  
## 1256 ATOM 1256 CA <NA> VAL A 164 <NA> 6.785 2.908 -19.578  
## 1257 ATOM 1257 C <NA> VAL A 164 <NA> 7.927 1.908 -19.662  
## 1258 ATOM 1258 O <NA> VAL A 164 <NA> 7.876 0.853 -19.029  
## 1259 ATOM 1259 CB <NA> VAL A 164 <NA> 6.044 2.970 -20.940  
## 1260 ATOM 1260 CG1 <NA> VAL A 164 <NA> 5.581 1.579 -21.380  
## 1261 ATOM 1261 CG2 <NA> VAL A 164 <NA> 4.849 3.876 -20.825  
## 1262 ATOM 1262 N <NA> ARG A 165 <NA> 8.968 2.244 -20.412  
## 1263 ATOM 1263 CA <NA> ARG A 165 <NA> 10.107 1.349 -20.547  
## 1264 ATOM 1264 C <NA> ARG A 165 <NA> 10.772 0.989 -19.219  
## 1265 ATOM 1265 O <NA> ARG A 165 <NA> 11.308 -0.107 -19.067  
## 1266 ATOM 1266 CB <NA> ARG A 165 <NA> 11.116 1.922 -21.526  
## 1267 ATOM 1267 CG <NA> ARG A 165 <NA> 10.627 1.835 -22.941  
## 1268 ATOM 1268 CD <NA> ARG A 165 <NA> 11.782 1.568 -23.884  
## 1269 ATOM 1269 NE <NA> ARG A 165 <NA> 11.329 1.024 -25.161  
## 1270 ATOM 1270 CZ <NA> ARG A 165 <NA> 11.159 1.750 -26.254  
## 1271 ATOM 1271 NH1 <NA> ARG A 165 <NA> 11.400 3.053 -26.222  
## 1272 ATOM 1272 NH2 <NA> ARG A 165 <NA> 10.743 1.176 -27.375  
## 1273 ATOM 1273 N <NA> LYS A 166 <NA> 10.713 1.897 -18.254  
## 1274 ATOM 1274 CA <NA> LYS A 166 <NA> 11.286 1.660 -16.939  
## 1275 ATOM 1275 C <NA> LYS A 166 <NA> 10.416 0.669 -16.173  
## 1276 ATOM 1276 O <NA> LYS A 166 <NA> 10.929 -0.251 -15.541  
## 1277 ATOM 1277 CB <NA> LYS A 166 <NA> 11.363 2.960 -16.175  
## 1278 ATOM 1278 CG <NA> LYS A 166 <NA> 12.762 3.402 -15.823  
## 1279 ATOM 1279 CD <NA> LYS A 166 <NA> 12.730 4.887 -15.465  
## 1280 ATOM 1280 CE <NA> LYS A 166 <NA> 11.525 5.236 -14.565  
## 1281 ATOM 1281 NZ <NA> LYS A 166 <NA> 11.145 6.686 -14.614  
## 1282 ATOM 1282 N <NA> ARG A 167 <NA> 9.102 0.850 -16.222  
## 1283 ATOM 1283 CA <NA> ARG A 167 <NA> 8.203 -0.073 -15.550  
## 1284 ATOM 1284 C <NA> ARG A 167 <NA> 8.415 -1.506 -16.038  
## 1285 ATOM 1285 O <NA> ARG A 167 <NA> 8.424 -2.453 -15.250  
## 1286 ATOM 1286 CB <NA> ARG A 167 <NA> 6.756 0.311 -15.816  
## 1287 ATOM 1287 CG <NA> ARG A 167 <NA> 6.224 1.402 -14.924  
## 1288 ATOM 1288 CD <NA> ARG A 167 <NA> 4.714 1.223 -14.705  
## 1289 ATOM 1289 NE <NA> ARG A 167 <NA> 3.942 1.425 -15.930  
## 1290 ATOM 1290 CZ <NA> ARG A 167 <NA> 3.354 2.570 -16.262  
## 1291 ATOM 1291 NH1 <NA> ARG A 167 <NA> 3.426 3.616 -15.451  
## 1292 ATOM 1292 NH2 <NA> ARG A 167 <NA> 2.680 2.665 -17.399  
## 1293 ATOM 1293 N <NA> LEU A 168 <NA> 8.580 -1.666 -17.346  
## 1294 ATOM 1294 CA <NA> LEU A 168 <NA> 8.761 -2.980 -17.910  
## 1295 ATOM 1295 C <NA> LEU A 168 <NA> 10.058 -3.650 -17.537  
## 1296 ATOM 1296 O <NA> LEU A 168 <NA> 10.068 -4.863 -17.316  
## 1297 ATOM 1297 CB <NA> LEU A 168 <NA> 8.581 -2.950 -19.418  
## 1298 ATOM 1298 CG <NA> LEU A 168 <NA> 7.159 -2.716 -19.963  
## 1299 ATOM 1299 CD1 <NA> LEU A 168 <NA> 7.237 -2.459 -21.484  
## 1300 ATOM 1300 CD2 <NA> LEU A 168 <NA> 6.250 -3.896 -19.640  
## 1301 ATOM 1301 N <NA> VAL A 169 <NA> 11.160 -2.902 -17.471  
## 1302 ATOM 1302 CA <NA> VAL A 169 <NA> 12.440 -3.514 -17.081  
## 1303 ATOM 1303 C <NA> VAL A 169 <NA> 12.330 -3.986 -15.633  
## 1304 ATOM 1304 O <NA> VAL A 169 <NA> 12.645 -5.136 -15.294  
## 1305 ATOM 1305 CB <NA> VAL A 169 <NA> 13.660 -2.544 -17.217  
## 1306 ATOM 1306 CG1 <NA> VAL A 169 <NA> 13.444 -1.276 -16.418  
## 1307 ATOM 1307 CG2 <NA> VAL A 169 <NA> 14.931 -3.228 -16.720  
## 1308 ATOM 1308 N <NA> GLU A 170 <NA> 11.778 -3.101 -14.821  
## 1309 ATOM 1309 CA <NA> GLU A 170 <NA> 11.557 -3.317 -13.412  
## 1310 ATOM 1310 C <NA> GLU A 170 <NA> 10.740 -4.608 -13.205  
## 1311 ATOM 1311 O <NA> GLU A 170 <NA> 11.029 -5.427 -12.309  
## 1312 ATOM 1312 CB <NA> GLU A 170 <NA> 10.803 -2.096 -12.896  
## 1313 ATOM 1313 CG <NA> GLU A 170 <NA> 11.109 -1.692 -11.482  
## 1314 ATOM 1314 CD <NA> GLU A 170 <NA> 9.993 -2.063 -10.530  
## 1315 ATOM 1315 OE1 <NA> GLU A 170 <NA> 8.811 -1.821 -10.882  
## 1316 ATOM 1316 OE2 <NA> GLU A 170 <NA> 10.300 -2.589 -9.432  
## 1317 ATOM 1317 N <NA> TYR A 171 <NA> 9.730 -4.774 -14.059  
## 1318 ATOM 1318 CA <NA> TYR A 171 <NA> 8.844 -5.924 -14.041  
## 1319 ATOM 1319 C <NA> TYR A 171 <NA> 9.596 -7.193 -14.407  
## 1320 ATOM 1320 O <NA> TYR A 171 <NA> 9.454 -8.228 -13.759  
## 1321 ATOM 1321 CB <NA> TYR A 171 <NA> 7.682 -5.701 -15.020  
## 1322 ATOM 1322 CG <NA> TYR A 171 <NA> 6.841 -6.934 -15.244  
## 1323 ATOM 1323 CD1 <NA> TYR A 171 <NA> 5.899 -7.334 -14.310  
## 1324 ATOM 1324 CD2 <NA> TYR A 171 <NA> 7.044 -7.741 -16.362  
## 1325 ATOM 1325 CE1 <NA> TYR A 171 <NA> 5.178 -8.524 -14.477  
## 1326 ATOM 1326 CE2 <NA> TYR A 171 <NA> 6.334 -8.928 -16.539  
## 1327 ATOM 1327 CZ <NA> TYR A 171 <NA> 5.402 -9.319 -15.585  
## 1328 ATOM 1328 OH <NA> TYR A 171 <NA> 4.718 -10.515 -15.765  
## 1329 ATOM 1329 N <NA> HIS A 172 <NA> 10.408 -7.114 -15.443  
## 1330 ATOM 1330 CA <NA> HIS A 172 <NA> 11.163 -8.267 -15.892  
## 1331 ATOM 1331 C <NA> HIS A 172 <NA> 12.279 -8.753 -14.993  
## 1332 ATOM 1332 O <NA> HIS A 172 <NA> 12.481 -9.965 -14.879  
## 1333 ATOM 1333 CB <NA> HIS A 172 <NA> 11.699 -8.024 -17.280  
## 1334 ATOM 1334 CG <NA> HIS A 172 <NA> 10.654 -8.125 -18.327  
## 1335 ATOM 1335 ND1 <NA> HIS A 172 <NA> 10.048 -9.317 -18.643  
## 1336 ATOM 1336 CD2 <NA> HIS A 172 <NA> 10.070 -7.185 -19.101  
## 1337 ATOM 1337 CE1 <NA> HIS A 172 <NA> 9.130 -9.111 -19.567  
## 1338 ATOM 1338 NE2 <NA> HIS A 172 <NA> 9.123 -7.824 -19.862  
## 1339 ATOM 1339 N <NA> GLN A 173 <NA> 13.039 -7.846 -14.388  
## 1340 ATOM 1340 CA <NA> GLN A 173 <NA> 14.107 -8.297 -13.497  
## 1341 ATOM 1341 C <NA> GLN A 173 <NA> 13.486 -9.025 -12.283  
## 1342 ATOM 1342 O <NA> GLN A 173 <NA> 14.040 -9.988 -11.748  
## 1343 ATOM 1343 CB <NA> GLN A 173 <NA> 14.976 -7.115 -13.027  
## 1344 ATOM 1344 CG <NA> GLN A 173 <NA> 14.244 -6.092 -12.144  
## 1345 ATOM 1345 CD <NA> GLN A 173 <NA> 15.124 -4.923 -11.667  
## 1346 ATOM 1346 OE1 <NA> GLN A 173 <NA> 15.010 -4.478 -10.521  
## 1347 ATOM 1347 NE2 <NA> GLN A 173 <NA> 15.974 -4.405 -12.553  
## 1348 ATOM 1348 N <NA> MET A 174 <NA> 12.297 -8.574 -11.899  
## 1349 ATOM 1349 CA <NA> MET A 174 <NA> 11.551 -9.104 -10.763  
## 1350 ATOM 1350 C <NA> MET A 174 <NA> 10.787 -10.413 -11.040  
## 1351 ATOM 1351 O <NA> MET A 174 <NA> 10.794 -11.339 -10.214  
## 1352 ATOM 1352 CB <NA> MET A 174 <NA> 10.615 -7.989 -10.278  
## 1353 ATOM 1353 CG <NA> MET A 174 <NA> 9.726 -8.299 -9.116  
## 1354 ATOM 1354 SD <NA> MET A 174 <NA> 8.965 -6.754 -8.564  
## 1355 ATOM 1355 CE <NA> MET A 174 <NA> 7.217 -7.003 -9.038  
## 1356 ATOM 1356 N <NA> THR A 175 <NA> 10.222 -10.534 -12.236  
## 1357 ATOM 1357 CA <NA> THR A 175 <NA> 9.443 -11.711 -12.583  
## 1358 ATOM 1358 C <NA> THR A 175 <NA> 10.161 -12.826 -13.306  
## 1359 ATOM 1359 O <NA> THR A 175 <NA> 9.667 -13.953 -13.349  
## 1360 ATOM 1360 CB <NA> THR A 175 <NA> 8.207 -11.311 -13.381  
## 1361 ATOM 1361 OG1 <NA> THR A 175 <NA> 7.661 -10.127 -12.795  
## 1362 ATOM 1362 CG2 <NA> THR A 175 <NA> 7.150 -12.384 -13.304  
## 1363 ATOM 1363 N <NA> ALA A 176 <NA> 11.338 -12.545 -13.846  
## 1364 ATOM 1364 CA <NA> ALA A 176 <NA> 12.084 -13.570 -14.552  
## 1365 ATOM 1365 C <NA> ALA A 176 <NA> 12.313 -14.845 -13.702  
## 1366 ATOM 1366 O <NA> ALA A 176 <NA> 12.000 -15.947 -14.153  
## 1367 ATOM 1367 CB <NA> ALA A 176 <NA> 13.418 -12.986 -15.088  
## 1368 ATOM 1368 N <NA> PRO A 177 <NA> 12.846 -14.719 -12.464  
## 1369 ATOM 1369 CA <NA> PRO A 177 <NA> 13.053 -15.945 -11.666  
## 1370 ATOM 1370 C <NA> PRO A 177 <NA> 11.775 -16.617 -11.131  
## 1371 ATOM 1371 O <NA> PRO A 177 <NA> 11.775 -17.815 -10.822  
## 1372 ATOM 1372 CB <NA> PRO A 177 <NA> 14.004 -15.491 -10.558  
## 1373 ATOM 1373 CG <NA> PRO A 177 <NA> 13.695 -14.049 -10.391  
## 1374 ATOM 1374 CD <NA> PRO A 177 <NA> 13.467 -13.552 -11.806  
## 1375 ATOM 1375 N <NA> LEU A 178 <NA> 10.673 -15.866 -11.078  
## 1376 ATOM 1376 CA <NA> LEU A 178 <NA> 9.391 -16.417 -10.632  
## 1377 ATOM 1377 C <NA> LEU A 178 <NA> 8.831 -17.330 -11.709  
## 1378 ATOM 1378 O <NA> LEU A 178 <NA> 8.277 -18.396 -11.431  
## 1379 ATOM 1379 CB <NA> LEU A 178 <NA> 8.411 -15.296 -10.359  
## 1380 ATOM 1380 CG <NA> LEU A 178 <NA> 7.060 -15.800 -9.896  
## 1381 ATOM 1381 CD1 <NA> LEU A 178 <NA> 7.172 -16.639 -8.624  
## 1382 ATOM 1382 CD2 <NA> LEU A 178 <NA> 6.235 -14.588 -9.666  
## 1383 ATOM 1383 N <NA> ILE A 179 <NA> 8.984 -16.896 -12.956  
## 1384 ATOM 1384 CA <NA> ILE A 179 <NA> 8.528 -17.683 -14.088  
## 1385 ATOM 1385 C <NA> ILE A 179 <NA> 9.331 -18.968 -14.057  
## 1386 ATOM 1386 O <NA> ILE A 179 <NA> 8.780 -20.063 -14.239  
## 1387 ATOM 1387 CB <NA> ILE A 179 <NA> 8.829 -16.967 -15.412  
## 1388 ATOM 1388 CG1 <NA> ILE A 179 <NA> 8.162 -15.606 -15.425  
## 1389 ATOM 1389 CG2 <NA> ILE A 179 <NA> 8.358 -17.813 -16.597  
## 1390 ATOM 1390 CD1 <NA> ILE A 179 <NA> 6.682 -15.685 -15.175  
## 1391 ATOM 1391 N <NA> GLY A 180 <NA> 10.642 -18.816 -13.821  
## 1392 ATOM 1392 CA <NA> GLY A 180 <NA> 11.552 -19.954 -13.763  
## 1393 ATOM 1393 C <NA> GLY A 180 <NA> 11.206 -20.871 -12.608  
## 1394 ATOM 1394 O <NA> GLY A 180 <NA> 11.333 -22.087 -12.694  
## 1395 ATOM 1395 N <NA> TYR A 181 <NA> 10.783 -20.269 -11.508  
## 1396 ATOM 1396 CA <NA> TYR A 181 <NA> 10.377 -21.026 -10.344  
## 1397 ATOM 1397 C <NA> TYR A 181 <NA> 9.166 -21.869 -10.735  
## 1398 ATOM 1398 O <NA> TYR A 181 <NA> 9.143 -23.083 -10.507  
## 1399 ATOM 1399 CB <NA> TYR A 181 <NA> 9.987 -20.064 -9.223  
## 1400 ATOM 1400 CG <NA> TYR A 181 <NA> 9.349 -20.732 -8.031  
## 1401 ATOM 1401 CD1 <NA> TYR A 181 <NA> 7.959 -20.921 -7.959  
## 1402 ATOM 1402 CD2 <NA> TYR A 181 <NA> 10.129 -21.166 -6.970  
## 1403 ATOM 1403 CE1 <NA> TYR A 181 <NA> 7.375 -21.522 -6.866  
## 1404 ATOM 1404 CE2 <NA> TYR A 181 <NA> 9.551 -21.769 -5.857  
## 1405 ATOM 1405 CZ <NA> TYR A 181 <NA> 8.176 -21.940 -5.809  
## 1406 ATOM 1406 OH <NA> TYR A 181 <NA> 7.622 -22.490 -4.674  
## 1407 ATOM 1407 N <NA> TYR A 182 <NA> 8.155 -21.225 -11.315  
## 1408 ATOM 1408 CA <NA> TYR A 182 <NA> 6.949 -21.944 -11.714  
## 1409 ATOM 1409 C <NA> TYR A 182 <NA> 7.150 -22.997 -12.796  
## 1410 ATOM 1410 O <NA> TYR A 182 <NA> 6.345 -23.922 -12.888  
## 1411 ATOM 1411 CB <NA> TYR A 182 <NA> 5.824 -20.986 -12.068  
## 1412 ATOM 1412 CG <NA> TYR A 182 <NA> 5.107 -20.480 -10.837  
## 1413 ATOM 1413 CD1 <NA> TYR A 182 <NA> 4.612 -21.371 -9.878  
## 1414 ATOM 1414 CD2 <NA> TYR A 182 <NA> 4.969 -19.118 -10.594  
## 1415 ATOM 1415 CE1 <NA> TYR A 182 <NA> 4.006 -20.914 -8.681  
## 1416 ATOM 1416 CE2 <NA> TYR A 182 <NA> 4.351 -18.653 -9.412  
## 1417 ATOM 1417 CZ <NA> TYR A 182 <NA> 3.882 -19.560 -8.457  
## 1418 ATOM 1418 OH <NA> TYR A 182 <NA> 3.327 -19.091 -7.272  
## 1419 ATOM 1419 N <NA> SER A 183 <NA> 8.181 -22.869 -13.634  
## 1420 ATOM 1420 CA <NA> SER A 183 <NA> 8.422 -23.921 -14.632  
## 1421 ATOM 1421 C <NA> SER A 183 <NA> 9.023 -25.129 -13.935  
## 1422 ATOM 1422 O <NA> SER A 183 <NA> 8.674 -26.256 -14.256  
## 1423 ATOM 1423 CB <NA> SER A 183 <NA> 9.371 -23.483 -15.731  
## 1424 ATOM 1424 OG <NA> SER A 183 <NA> 8.820 -22.409 -16.435  
## 1425 ATOM 1425 N <NA> LYS A 184 <NA> 9.929 -24.904 -12.983  
## 1426 ATOM 1426 CA <NA> LYS A 184 <NA> 10.539 -26.020 -12.265  
## 1427 ATOM 1427 C <NA> LYS A 184 <NA> 9.471 -26.752 -11.498  
## 1428 ATOM 1428 O <NA> LYS A 184 <NA> 9.492 -27.972 -11.410  
## 1429 ATOM 1429 CB <NA> LYS A 184 <NA> 11.670 -25.571 -11.333  
## 1430 ATOM 1430 CG <NA> LYS A 184 <NA> 13.077 -25.875 -11.894  
## 1431 ATOM 1431 CD <NA> LYS A 184 <NA> 14.184 -25.736 -10.832  
## 1432 ATOM 1432 CE <NA> LYS A 184 <NA> 15.580 -25.908 -11.438  
## 1433 ATOM 1433 NZ <NA> LYS A 184 <NA> 16.680 -25.564 -10.478  
## 1434 ATOM 1434 N <NA> GLU A 185 <NA> 8.512 -26.003 -10.971  
## 1435 ATOM 1435 CA <NA> GLU A 185 <NA> 7.403 -26.586 -10.232  
## 1436 ATOM 1436 C <NA> GLU A 185 <NA> 6.535 -27.397 -11.195  
## 1437 ATOM 1437 O <NA> GLU A 185 <NA> 6.105 -28.507 -10.884  
## 1438 ATOM 1438 CB <NA> GLU A 185 <NA> 6.573 -25.477 -9.604  
## 1439 ATOM 1439 CG <NA> GLU A 185 <NA> 7.184 -24.895 -8.376  
## 1440 ATOM 1440 CD <NA> GLU A 185 <NA> 7.262 -25.919 -7.282  
## 1441 ATOM 1441 OE1 <NA> GLU A 185 <NA> 6.221 -26.523 -6.951  
## 1442 ATOM 1442 OE2 <NA> GLU A 185 <NA> 8.369 -26.154 -6.773  
## 1443 ATOM 1443 N <NA> ALA A 186 <NA> 6.287 -26.835 -12.370  
## 1444 ATOM 1444 CA <NA> ALA A 186 <NA> 5.477 -27.492 -13.386  
## 1445 ATOM 1445 C <NA> ALA A 186 <NA> 6.102 -28.820 -13.764  
## 1446 ATOM 1446 O <NA> ALA A 186 <NA> 5.403 -29.829 -13.834  
## 1447 ATOM 1447 CB <NA> ALA A 186 <NA> 5.340 -26.594 -14.601  
## 1448 ATOM 1448 N <NA> GLU A 187 <NA> 7.422 -28.812 -13.986  
## 1449 ATOM 1449 CA <NA> GLU A 187 <NA> 8.198 -30.014 -14.339  
## 1450 ATOM 1450 C <NA> GLU A 187 <NA> 8.194 -31.002 -13.170  
## 1451 ATOM 1451 O <NA> GLU A 187 <NA> 8.260 -32.205 -13.365  
## 1452 ATOM 1452 CB <NA> GLU A 187 <NA> 9.650 -29.655 -14.735  
## 1453 ATOM 1453 CG <NA> GLU A 187 <NA> 9.822 -29.039 -16.160  
## 1454 ATOM 1454 CD <NA> GLU A 187 <NA> 11.211 -28.379 -16.427  
## 1455 ATOM 1455 OE1 <NA> GLU A 187 <NA> 12.247 -28.905 -15.950  
## 1456 ATOM 1456 OE2 <NA> GLU A 187 <NA> 11.259 -27.333 -17.133  
## 1457 ATOM 1457 N <NA> ALA A 188 <NA> 8.083 -30.486 -11.956  
## 1458 ATOM 1458 CA <NA> ALA A 188 <NA> 8.038 -31.325 -10.781  
## 1459 ATOM 1459 C <NA> ALA A 188 <NA> 6.648 -31.925 -10.633  
## 1460 ATOM 1460 O <NA> ALA A 188 <NA> 6.425 -32.775 -9.778  
## 1461 ATOM 1461 CB <NA> ALA A 188 <NA> 8.382 -30.511 -9.551  
## 1462 ATOM 1462 N <NA> GLY A 189 <NA> 5.704 -31.450 -11.440  
## 1463 ATOM 1463 CA <NA> GLY A 189 <NA> 4.339 -31.962 -11.390  
## 1464 ATOM 1464 C <NA> GLY A 189 <NA> 3.459 -31.333 -10.324  
## 1465 ATOM 1465 O <NA> GLY A 189 <NA> 2.335 -31.786 -10.089  
## 1466 ATOM 1466 N <NA> ASN A 190 <NA> 3.949 -30.254 -9.715  
## 1467 ATOM 1467 CA <NA> ASN A 190 <NA> 3.218 -29.550 -8.655  
## 1468 ATOM 1468 C <NA> ASN A 190 <NA> 2.159 -28.546 -9.137  
## 1469 ATOM 1469 O <NA> ASN A 190 <NA> 1.306 -28.099 -8.354  
## 1470 ATOM 1470 CB <NA> ASN A 190 <NA> 4.202 -28.836 -7.710  
## 1471 ATOM 1471 CG <NA> ASN A 190 <NA> 4.907 -29.791 -6.746  
## 1472 ATOM 1472 OD1 <NA> ASN A 190 <NA> 4.269 -30.606 -6.073  
## 1473 ATOM 1473 ND2 <NA> ASN A 190 <NA> 6.230 -29.675 -6.666  
## 1474 ATOM 1474 N <NA> THR A 191 <NA> 2.214 -28.193 -10.417  
## 1475 ATOM 1475 CA <NA> THR A 191 <NA> 1.293 -27.230 -10.992  
## 1476 ATOM 1476 C <NA> THR A 191 <NA> 1.523 -27.295 -12.481  
## 1477 ATOM 1477 O <NA> THR A 191 <NA> 2.388 -28.052 -12.939  
## 1478 ATOM 1478 CB <NA> THR A 191 <NA> 1.601 -25.817 -10.464  
## 1479 ATOM 1479 OG1 <NA> THR A 191 <NA> 0.610 -24.893 -10.917  
## 1480 ATOM 1480 CG2 <NA> THR A 191 <NA> 2.976 -25.353 -10.913  
## 1481 ATOM 1481 N <NA> LYS A 192 <NA> 0.695 -26.594 -13.248  
## 1482 ATOM 1482 CA <NA> LYS A 192 <NA> 0.851 -26.553 -14.706  
## 1483 ATOM 1483 C <NA> LYS A 192 <NA> 1.141 -25.109 -15.085  
## 1484 ATOM 1484 O <NA> LYS A 192 <NA> 0.479 -24.195 -14.619  
## 1485 ATOM 1485 CB <NA> LYS A 192 <NA> -0.409 -27.041 -15.444  
## 1486 ATOM 1486 CG <NA> LYS A 192 <NA> -0.716 -28.532 -15.305  
## 1487 ATOM 1487 CD <NA> LYS A 192 <NA> -1.678 -28.843 -14.134  
## 1488 ATOM 1488 CE <NA> LYS A 192 <NA> -3.153 -28.883 -14.580  
## 1489 ATOM 1489 NZ <NA> LYS A 192 <NA> -4.138 -29.125 -13.471  
## 1490 ATOM 1490 N <NA> TYR A 193 <NA> 2.153 -24.894 -15.900  
## 1491 ATOM 1491 CA <NA> TYR A 193 <NA> 2.499 -23.551 -16.307  
## 1492 ATOM 1492 C <NA> TYR A 193 <NA> 2.250 -23.437 -17.807  
## 1493 ATOM 1493 O <NA> TYR A 193 <NA> 2.465 -24.400 -18.535  
## 1494 ATOM 1494 CB <NA> TYR A 193 <NA> 3.971 -23.290 -15.951  
## 1495 ATOM 1495 CG <NA> TYR A 193 <NA> 4.549 -22.097 -16.641  
## 1496 ATOM 1496 CD1 <NA> TYR A 193 <NA> 4.256 -20.799 -16.230  
## 1497 ATOM 1497 CD2 <NA> TYR A 193 <NA> 5.327 -22.266 -17.772  
## 1498 ATOM 1498 CE1 <NA> TYR A 193 <NA> 4.729 -19.697 -16.959  
## 1499 ATOM 1499 CE2 <NA> TYR A 193 <NA> 5.796 -21.187 -18.490  
## 1500 ATOM 1500 CZ <NA> TYR A 193 <NA> 5.500 -19.915 -18.091  
## 1501 ATOM 1501 OH <NA> TYR A 193 <NA> 5.993 -18.892 -18.874  
## 1502 ATOM 1502 N <NA> ALA A 194 <NA> 1.763 -22.298 -18.278  
## 1503 ATOM 1503 CA <NA> ALA A 194 <NA> 1.534 -22.156 -19.717  
## 1504 ATOM 1504 C <NA> ALA A 194 <NA> 1.722 -20.723 -20.148  
## 1505 ATOM 1505 O <NA> ALA A 194 <NA> 1.369 -19.819 -19.411  
## 1506 ATOM 1506 CB <NA> ALA A 194 <NA> 0.134 -22.651 -20.103  
## 1507 ATOM 1507 N <NA> LYS A 195 <NA> 2.332 -20.517 -21.309  
## 1508 ATOM 1508 CA <NA> LYS A 195 <NA> 2.555 -19.171 -21.832  
## 1509 ATOM 1509 C <NA> LYS A 195 <NA> 1.497 -18.899 -22.896  
## 1510 ATOM 1510 O <NA> LYS A 195 <NA> 1.286 -19.711 -23.792  
## 1511 ATOM 1511 CB <NA> LYS A 195 <NA> 3.954 -19.047 -22.427  
## 1512 ATOM 1512 CG <NA> LYS A 195 <NA> 4.236 -17.687 -23.059  
## 1513 ATOM 1513 CD <NA> LYS A 195 <NA> 5.502 -17.017 -22.510  
## 1514 ATOM 1514 CE <NA> LYS A 195 <NA> 6.779 -17.815 -22.769  
## 1515 ATOM 1515 NZ <NA> LYS A 195 <NA> 7.039 -18.869 -21.736  
## 1516 ATOM 1516 N <NA> VAL A 196 <NA> 0.880 -17.730 -22.825  
## 1517 ATOM 1517 CA <NA> VAL A 196 <NA> -0.205 -17.357 -23.721  
## 1518 ATOM 1518 C <NA> VAL A 196 <NA> 0.193 -16.182 -24.590  
## 1519 ATOM 1519 O <NA> VAL A 196 <NA> 0.638 -15.158 -24.084  
## 1520 ATOM 1520 CB <NA> VAL A 196 <NA> -1.473 -16.997 -22.864  
## 1521 ATOM 1521 CG1 <NA> VAL A 196 <NA> -2.439 -16.129 -23.616  
## 1522 ATOM 1522 CG2 <NA> VAL A 196 <NA> -2.169 -18.258 -22.399  
## 1523 ATOM 1523 N <NA> ASP A 197 <NA> 0.050 -16.323 -25.902  
## 1524 ATOM 1524 CA <NA> ASP A 197 <NA> 0.406 -15.231 -26.795  
## 1525 ATOM 1525 C <NA> ASP A 197 <NA> -0.721 -14.227 -26.707  
## 1526 ATOM 1526 O <NA> ASP A 197 <NA> -1.811 -14.478 -27.173  
## 1527 ATOM 1527 CB <NA> ASP A 197 <NA> 0.589 -15.738 -28.238  
## 1528 ATOM 1528 CG <NA> ASP A 197 <NA> 1.167 -14.664 -29.194  
## 1529 ATOM 1529 OD1 <NA> ASP A 197 <NA> 1.892 -13.746 -28.748  
## 1530 ATOM 1530 OD2 <NA> ASP A 197 <NA> 0.918 -14.759 -30.414  
## 1531 ATOM 1531 N <NA> GLY A 198 <NA> -0.470 -13.123 -26.032  
## 1532 ATOM 1532 CA <NA> GLY A 198 <NA> -1.480 -12.100 -25.886  
## 1533 ATOM 1533 C <NA> GLY A 198 <NA> -1.593 -11.200 -27.092  
## 1534 ATOM 1534 O <NA> GLY A 198 <NA> -2.343 -10.226 -27.081  
## 1535 ATOM 1535 N <NA> THR A 199 <NA> -0.829 -11.508 -28.132  
## 1536 ATOM 1536 CA <NA> THR A 199 <NA> -0.846 -10.720 -29.359  
## 1537 ATOM 1537 C <NA> THR A 199 <NA> -1.840 -11.289 -30.387  
## 1538 ATOM 1538 O <NA> THR A 199 <NA> -1.817 -10.909 -31.552  
## 1539 ATOM 1539 CB <NA> THR A 199 <NA> 0.549 -10.692 -29.997  
## 1540 ATOM 1540 OG1 <NA> THR A 199 <NA> 0.870 -12.007 -30.465  
## 1541 ATOM 1541 CG2 <NA> THR A 199 <NA> 1.604 -10.245 -28.984  
## 1542 ATOM 1542 N <NA> LYS A 200 <NA> -2.643 -12.267 -29.980  
## 1543 ATOM 1543 CA <NA> LYS A 200 <NA> -3.634 -12.872 -30.862  
## 1544 ATOM 1544 C <NA> LYS A 200 <NA> -5.009 -12.275 -30.638  
## 1545 ATOM 1545 O <NA> LYS A 200 <NA> -5.259 -11.603 -29.638  
## 1546 ATOM 1546 CB <NA> LYS A 200 <NA> -3.787 -14.349 -30.581  
## 1547 ATOM 1547 CG <NA> LYS A 200 <NA> -2.723 -15.192 -31.107  
## 1548 ATOM 1548 CD <NA> LYS A 200 <NA> -3.154 -16.584 -30.830  
## 1549 ATOM 1549 CE <NA> LYS A 200 <NA> -2.137 -17.571 -31.279  
## 1550 ATOM 1550 NZ <NA> LYS A 200 <NA> -2.719 -18.925 -31.120  
## 1551 ATOM 1551 N <NA> PRO A 201 <NA> -5.927 -12.510 -31.583  
## 1552 ATOM 1552 CA <NA> PRO A 201 <NA> -7.282 -11.980 -31.421  
## 1553 ATOM 1553 C <NA> PRO A 201 <NA> -7.880 -12.539 -30.140  
## 1554 ATOM 1554 O <NA> PRO A 201 <NA> -7.697 -13.717 -29.834  
## 1555 ATOM 1555 CB <NA> PRO A 201 <NA> -8.020 -12.519 -32.666  
## 1556 ATOM 1556 CG <NA> PRO A 201 <NA> -7.125 -13.652 -33.193  
## 1557 ATOM 1557 CD <NA> PRO A 201 <NA> -5.748 -13.106 -32.921  
## 1558 ATOM 1558 N <NA> VAL A 202 <NA> -8.595 -11.693 -29.408  
## 1559 ATOM 1559 CA <NA> VAL A 202 <NA> -9.230 -12.083 -28.161  
## 1560 ATOM 1560 C <NA> VAL A 202 <NA> -9.951 -13.414 -28.312  
## 1561 ATOM 1561 O <NA> VAL A 202 <NA> -9.889 -14.273 -27.425  
## 1562 ATOM 1562 CB <NA> VAL A 202 <NA> -10.178 -10.968 -27.676  
## 1563 ATOM 1563 CG1 <NA> VAL A 202 <NA> -11.088 -11.455 -26.561  
## 1564 ATOM 1564 CG2 <NA> VAL A 202 <NA> -9.355 -9.795 -27.187  
## 1565 ATOM 1565 N <NA> ALA A 203 <NA> -10.559 -13.615 -29.481  
## 1566 ATOM 1566 CA <NA> ALA A 203 <NA> -11.280 -14.851 -29.764  
## 1567 ATOM 1567 C <NA> ALA A 203 <NA> -10.326 -16.021 -29.938  
## 1568 ATOM 1568 O <NA> ALA A 203 <NA> -10.704 -17.180 -29.718  
## 1569 ATOM 1569 CB <NA> ALA A 203 <NA> -12.142 -14.695 -30.989  
## 1570 ATOM 1570 N <NA> GLU A 204 <NA> -9.104 -15.747 -30.382  
## 1571 ATOM 1571 CA <NA> GLU A 204 <NA> -8.168 -16.841 -30.534  
## 1572 ATOM 1572 C <NA> GLU A 204 <NA> -7.574 -17.170 -29.191  
## 1573 ATOM 1573 O <NA> GLU A 204 <NA> -7.516 -18.337 -28.821  
## 1574 ATOM 1574 CB <NA> GLU A 204 <NA> -7.083 -16.538 -31.546  
## 1575 ATOM 1575 CG <NA> GLU A 204 <NA> -6.488 -17.813 -32.114  
## 1576 ATOM 1576 CD <NA> GLU A 204 <NA> -5.650 -17.576 -33.349  
## 1577 ATOM 1577 OE1 <NA> GLU A 204 <NA> -5.881 -16.568 -34.057  
## 1578 ATOM 1578 OE2 <NA> GLU A 204 <NA> -4.760 -18.410 -33.614  
## 1579 ATOM 1579 N <NA> VAL A 205 <NA> -7.209 -16.145 -28.422  
## 1580 ATOM 1580 CA <NA> VAL A 205 <NA> -6.640 -16.359 -27.091  
## 1581 ATOM 1581 C <NA> VAL A 205 <NA> -7.611 -17.183 -26.242  
## 1582 ATOM 1582 O <NA> VAL A 205 <NA> -7.222 -18.163 -25.590  
## 1583 ATOM 1583 CB <NA> VAL A 205 <NA> -6.383 -15.045 -26.375  
## 1584 ATOM 1584 CG1 <NA> VAL A 205 <NA> -5.819 -15.325 -25.006  
## 1585 ATOM 1585 CG2 <NA> VAL A 205 <NA> -5.426 -14.199 -27.162  
## 1586 ATOM 1586 N <NA> ARG A 206 <NA> -8.879 -16.781 -26.277  
## 1587 ATOM 1587 CA <NA> ARG A 206 <NA> -9.942 -17.465 -25.555  
## 1588 ATOM 1588 C <NA> ARG A 206 <NA> -9.970 -18.933 -25.990  
## 1589 ATOM 1589 O <NA> ARG A 206 <NA> -10.055 -19.841 -25.162  
## 1590 ATOM 1590 CB <NA> ARG A 206 <NA> -11.262 -16.770 -25.867  
## 1591 ATOM 1591 CG <NA> ARG A 206 <NA> -12.436 -17.210 -25.042  
## 1592 ATOM 1592 CD <NA> ARG A 206 <NA> -13.457 -17.938 -25.910  
## 1593 ATOM 1593 NE <NA> ARG A 206 <NA> -14.746 -17.254 -25.936  
## 1594 ATOM 1594 CZ <NA> ARG A 206 <NA> -15.876 -17.770 -25.457  
## 1595 ATOM 1595 NH1 <NA> ARG A 206 <NA> -15.887 -18.982 -24.907  
## 1596 ATOM 1596 NH2 <NA> ARG A 206 <NA> -17.003 -17.073 -25.525  
## 1597 ATOM 1597 N <NA> ALA A 207 <NA> -9.842 -19.171 -27.291  
## 1598 ATOM 1598 CA <NA> ALA A 207 <NA> -9.823 -20.528 -27.818  
## 1599 ATOM 1599 C <NA> ALA A 207 <NA> -8.654 -21.266 -27.209  
## 1600 ATOM 1600 O <NA> ALA A 207 <NA> -8.808 -22.385 -26.745  
## 1601 ATOM 1601 CB <NA> ALA A 207 <NA> -9.689 -20.504 -29.319  
## 1602 ATOM 1602 N <NA> ASP A 208 <NA> -7.484 -20.635 -27.197  
## 1603 ATOM 1603 CA <NA> ASP A 208 <NA> -6.301 -21.256 -26.621  
## 1604 ATOM 1604 C <NA> ASP A 208 <NA> -6.494 -21.609 -25.158  
## 1605 ATOM 1605 O <NA> ASP A 208 <NA> -6.120 -22.707 -24.734  
## 1606 ATOM 1606 CB <NA> ASP A 208 <NA> -5.092 -20.349 -26.742  
## 1607 ATOM 1607 CG <NA> ASP A 208 <NA> -4.490 -20.363 -28.115  
## 1608 ATOM 1608 OD1 <NA> ASP A 208 <NA> -4.740 -21.323 -28.885  
## 1609 ATOM 1609 OD2 <NA> ASP A 208 <NA> -3.748 -19.405 -28.413  
## 1610 ATOM 1610 N <NA> LEU A 209 <NA> -7.072 -20.684 -24.388  
## 1611 ATOM 1611 CA <NA> LEU A 209 <NA> -7.317 -20.913 -22.976  
## 1612 ATOM 1612 C <NA> LEU A 209 <NA> -8.151 -22.142 -22.677  
## 1613 ATOM 1613 O <NA> LEU A 209 <NA> -7.921 -22.841 -21.692  
## 1614 ATOM 1614 CB <NA> LEU A 209 <NA> -7.956 -19.694 -22.360  
## 1615 ATOM 1615 CG <NA> LEU A 209 <NA> -6.861 -18.672 -22.147  
## 1616 ATOM 1616 CD1 <NA> LEU A 209 <NA> -7.387 -17.573 -21.284  
## 1617 ATOM 1617 CD2 <NA> LEU A 209 <NA> -5.667 -19.347 -21.476  
## 1618 ATOM 1618 N <NA> GLU A 210 <NA> -9.137 -22.409 -23.514  
## 1619 ATOM 1619 CA <NA> GLU A 210 <NA> -9.965 -23.575 -23.311  
## 1620 ATOM 1620 C <NA> GLU A 210 <NA> -9.170 -24.847 -23.565  
## 1621 ATOM 1621 O <NA> GLU A 210 <NA> -9.384 -25.856 -22.906  
## 1622 ATOM 1622 CB <NA> GLU A 210 <NA> -11.183 -23.516 -24.212  
## 1623 ATOM 1623 CG <NA> GLU A 210 <NA> -12.162 -22.441 -23.801  
## 1624 ATOM 1624 CD <NA> GLU A 210 <NA> -13.543 -22.640 -24.397  
## 1625 ATOM 1625 OE1 <NA> GLU A 210 <NA> -14.293 -23.514 -23.896  
## 1626 ATOM 1626 OE2 <NA> GLU A 210 <NA> -13.878 -21.912 -25.358  
## 1627 ATOM 1627 N <NA> LYS A 211 <NA> -8.238 -24.798 -24.508  
## 1628 ATOM 1628 CA <NA> LYS A 211 <NA> -7.420 -25.965 -24.825  
## 1629 ATOM 1629 C <NA> LYS A 211 <NA> -6.303 -26.183 -23.794  
## 1630 ATOM 1630 O <NA> LYS A 211 <NA> -5.577 -27.170 -23.848  
## 1631 ATOM 1631 CB <NA> LYS A 211 <NA> -6.827 -25.833 -26.234  
## 1632 ATOM 1632 CG <NA> LYS A 211 <NA> -7.816 -26.118 -27.383  
## 1633 ATOM 1633 CD <NA> LYS A 211 <NA> -7.782 -25.043 -28.497  
## 1634 ATOM 1634 CE <NA> LYS A 211 <NA> -6.390 -24.848 -29.128  
## 1635 ATOM 1635 NZ <NA> LYS A 211 <NA> -6.368 -23.696 -30.091  
## 1636 ATOM 1636 N <NA> ILE A 212 <NA> -6.152 -25.242 -22.872  
## 1637 ATOM 1637 CA <NA> ILE A 212 <NA> -5.132 -25.335 -21.828  
## 1638 ATOM 1638 C <NA> ILE A 212 <NA> -5.769 -25.753 -20.508  
## 1639 ATOM 1639 O <NA> ILE A 212 <NA> -5.216 -26.572 -19.786  
## 1640 ATOM 1640 CB <NA> ILE A 212 <NA> -4.408 -23.956 -21.607  
## 1641 ATOM 1641 CG1 <NA> ILE A 212 <NA> -3.402 -23.675 -22.726  
## 1642 ATOM 1642 CG2 <NA> ILE A 212 <NA> -3.723 -23.905 -20.243  
## 1643 ATOM 1643 CD1 <NA> ILE A 212 <NA> -2.764 -22.311 -22.626  
## 1644 ATOM 1644 N <NA> LEU A 213 <NA> -6.961 -25.226 -20.239  
## 1645 ATOM 1645 CA <NA> LEU A 213 <NA> -7.671 -25.459 -18.988  
## 1646 ATOM 1646 C <NA> LEU A 213 <NA> -8.693 -26.586 -18.936  
## 1647 ATOM 1647 O <NA> LEU A 213 <NA> -8.768 -27.324 -17.940  
## 1648 ATOM 1648 CB <NA> LEU A 213 <NA> -8.354 -24.163 -18.570  
## 1649 ATOM 1649 CG <NA> LEU A 213 <NA> -7.367 -23.024 -18.484  
## 1650 ATOM 1650 CD1 <NA> LEU A 213 <NA> -8.074 -21.705 -18.338  
## 1651 ATOM 1651 CD2 <NA> LEU A 213 <NA> -6.431 -23.293 -17.346  
## 1652 ATOM 1652 N <NA> GLY A 214 <NA> -9.507 -26.685 -19.981  
## 1653 ATOM 1653 CA <NA> GLY A 214 <NA> -10.547 -27.696 -20.013  
## 1654 ATOM 1654 C <NA> GLY A 214 <NA> -11.696 -27.223 -19.131  
## 1655 ATOM 1655 O <NA> GLY A 214 <NA> -12.524 -26.410 -19.615  
## 1656 ATOM 1656 OXT <NA> GLY A 214 <NA> -11.742 -27.620 -17.940  
## 1657 ATOM 1658 N <NA> MET B 1 <NA> -12.005 26.032 10.335  
## 1658 ATOM 1659 CA <NA> MET B 1 <NA> -10.923 25.531 11.222  
## 1659 ATOM 1660 C <NA> MET B 1 <NA> -10.230 24.337 10.556  
## 1660 ATOM 1661 O <NA> MET B 1 <NA> -10.873 23.346 10.220  
## 1661 ATOM 1662 CB <NA> MET B 1 <NA> -11.533 25.126 12.567  
## 1662 ATOM 1663 CG <NA> MET B 1 <NA> -10.535 24.741 13.644  
## 1663 ATOM 1664 SD <NA> MET B 1 <NA> -9.444 26.082 14.089  
## 1664 ATOM 1665 CE <NA> MET B 1 <NA> -10.504 27.013 15.130  
## 1665 ATOM 1666 N <NA> ARG B 2 <NA> -8.936 24.453 10.288  
## 1666 ATOM 1667 CA <NA> ARG B 2 <NA> -8.218 23.350 9.673  
## 1667 ATOM 1668 C <NA> ARG B 2 <NA> -7.190 22.993 10.705  
## 1668 ATOM 1669 O <NA> ARG B 2 <NA> -6.390 23.834 11.104  
## 1669 ATOM 1670 CB <NA> ARG B 2 <NA> -7.579 23.807 8.386  
## 1670 ATOM 1671 CG <NA> ARG B 2 <NA> -8.599 24.218 7.370  
## 1671 ATOM 1672 CD <NA> ARG B 2 <NA> -7.997 25.173 6.382  
## 1672 ATOM 1673 NE <NA> ARG B 2 <NA> -8.464 24.887 5.031  
## 1673 ATOM 1674 CZ <NA> ARG B 2 <NA> -7.733 25.043 3.934  
## 1674 ATOM 1675 NH1 <NA> ARG B 2 <NA> -6.489 25.516 4.008  
## 1675 ATOM 1676 NH2 <NA> ARG B 2 <NA> -8.264 24.740 2.757  
## 1676 ATOM 1677 N <NA> ILE B 3 <NA> -7.237 21.752 11.159  
## 1677 ATOM 1678 CA <NA> ILE B 3 <NA> -6.373 21.292 12.227  
## 1678 ATOM 1679 C <NA> ILE B 3 <NA> -5.632 20.031 11.855  
## 1679 ATOM 1680 O <NA> ILE B 3 <NA> -6.176 19.184 11.181  
## 1680 ATOM 1681 CB <NA> ILE B 3 <NA> -7.262 20.975 13.449  
## 1681 ATOM 1682 CG1 <NA> ILE B 3 <NA> -7.823 22.257 14.064  
## 1682 ATOM 1683 CG2 <NA> ILE B 3 <NA> -6.531 20.150 14.477  
## 1683 ATOM 1684 CD1 <NA> ILE B 3 <NA> -9.119 22.014 14.806  
## 1684 ATOM 1685 N <NA> ILE B 4 <NA> -4.375 19.922 12.267  
## 1685 ATOM 1686 CA <NA> ILE B 4 <NA> -3.583 18.706 12.039  
## 1686 ATOM 1687 C <NA> ILE B 4 <NA> -3.406 18.108 13.439  
## 1687 ATOM 1688 O <NA> ILE B 4 <NA> -2.974 18.798 14.357  
## 1688 ATOM 1689 CB <NA> ILE B 4 <NA> -2.179 19.000 11.430  
## 1689 ATOM 1690 CG1 <NA> ILE B 4 <NA> -2.298 19.278 9.933  
## 1690 ATOM 1691 CG2 <NA> ILE B 4 <NA> -1.218 17.810 11.677  
## 1691 ATOM 1692 CD1 <NA> ILE B 4 <NA> -1.039 19.856 9.359  
## 1692 ATOM 1693 N <NA> LEU B 5 <NA> -3.787 16.850 13.606  
## 1693 ATOM 1694 CA <NA> LEU B 5 <NA> -3.693 16.182 14.889  
## 1694 ATOM 1695 C <NA> LEU B 5 <NA> -2.594 15.143 14.825  
## 1695 ATOM 1696 O <NA> LEU B 5 <NA> -2.735 14.141 14.112  
## 1696 ATOM 1697 CB <NA> LEU B 5 <NA> -5.032 15.515 15.207  
## 1697 ATOM 1698 CG <NA> LEU B 5 <NA> -5.168 15.012 16.636  
## 1698 ATOM 1699 CD1 <NA> LEU B 5 <NA> -5.124 16.164 17.618  
## 1699 ATOM 1700 CD2 <NA> LEU B 5 <NA> -6.453 14.248 16.777  
## 1700 ATOM 1701 N <NA> LEU B 6 <NA> -1.477 15.411 15.506  
## 1701 ATOM 1702 CA <NA> LEU B 6 <NA> -0.323 14.483 15.537  
## 1702 ATOM 1703 C <NA> LEU B 6 <NA> -0.269 13.808 16.917  
## 1703 ATOM 1704 O <NA> LEU B 6 <NA> -0.665 14.402 17.926  
## 1704 ATOM 1705 CB <NA> LEU B 6 <NA> 1.009 15.230 15.274  
## 1705 ATOM 1706 CG <NA> LEU B 6 <NA> 1.124 16.178 14.057  
## 1706 ATOM 1707 CD1 <NA> LEU B 6 <NA> 2.502 16.818 14.005  
## 1707 ATOM 1708 CD2 <NA> LEU B 6 <NA> 0.819 15.457 12.744  
## 1708 ATOM 1709 N <NA> GLY B 7 <NA> 0.206 12.574 16.969  
## 1709 ATOM 1710 CA <NA> GLY B 7 <NA> 0.283 11.871 18.235  
## 1710 ATOM 1711 C <NA> GLY B 7 <NA> 0.890 10.516 17.985  
## 1711 ATOM 1712 O <NA> GLY B 7 <NA> 0.747 9.972 16.893  
## 1712 ATOM 1713 N <NA> ALA B 8 <NA> 1.588 9.985 18.986  
## 1713 ATOM 1714 CA <NA> ALA B 8 <NA> 2.255 8.682 18.907  
## 1714 ATOM 1715 C <NA> ALA B 8 <NA> 1.304 7.536 18.700  
## 1715 ATOM 1716 O <NA> ALA B 8 <NA> 0.116 7.607 19.057  
## 1716 ATOM 1717 CB <NA> ALA B 8 <NA> 3.093 8.412 20.193  
## 1717 ATOM 1718 N <NA> PRO B 9 <NA> 1.789 6.467 18.059  
## 1718 ATOM 1719 CA <NA> PRO B 9 <NA> 0.845 5.364 17.893  
## 1719 ATOM 1720 C <NA> PRO B 9 <NA> 0.488 4.844 19.311  
## 1720 ATOM 1721 O <NA> PRO B 9 <NA> 1.368 4.422 20.079  
## 1721 ATOM 1722 CB <NA> PRO B 9 <NA> 1.652 4.359 17.050  
## 1722 ATOM 1723 CG <NA> PRO B 9 <NA> 3.141 4.754 17.271  
## 1723 ATOM 1724 CD <NA> PRO B 9 <NA> 3.038 6.243 17.298  
## 1724 ATOM 1725 N <NA> GLY B 10 <NA> -0.781 4.980 19.691  
## 1725 ATOM 1726 CA <NA> GLY B 10 <NA> -1.218 4.527 21.005  
## 1726 ATOM 1727 C <NA> GLY B 10 <NA> -1.338 5.614 22.066  
## 1727 ATOM 1728 O <NA> GLY B 10 <NA> -1.585 5.332 23.239  
## 1728 ATOM 1729 N <NA> ALA B 11 <NA> -1.138 6.863 21.674  
## 1729 ATOM 1730 CA <NA> ALA B 11 <NA> -1.243 7.952 22.615  
## 1730 ATOM 1731 C <NA> ALA B 11 <NA> -2.703 8.289 22.955  
## 1731 ATOM 1732 O <NA> ALA B 11 <NA> -2.954 8.922 23.969  
## 1732 ATOM 1733 CB <NA> ALA B 11 <NA> -0.518 9.175 22.088  
## 1733 ATOM 1734 N <NA> GLY B 12 <NA> -3.657 7.893 22.109  
## 1734 ATOM 1735 CA <NA> GLY B 12 <NA> -5.067 8.180 22.367  
## 1735 ATOM 1736 C <NA> GLY B 12 <NA> -5.597 9.551 21.942  
## 1736 ATOM 1737 O <NA> GLY B 12 <NA> -6.538 10.055 22.544  
## 1737 ATOM 1738 N <NA> LYS B 13 <NA> -5.043 10.131 20.874  
## 1738 ATOM 1739 CA <NA> LYS B 13 <NA> -5.471 11.450 20.366  
## 1739 ATOM 1740 C <NA> LYS B 13 <NA> -6.883 11.462 19.798  
## 1740 ATOM 1741 O <NA> LYS B 13 <NA> -7.518 12.514 19.723  
## 1741 ATOM 1742 CB <NA> LYS B 13 <NA> -4.507 11.961 19.289  
## 1742 ATOM 1743 CG <NA> LYS B 13 <NA> -3.946 10.872 18.418  
## 1743 ATOM 1744 CD <NA> LYS B 13 <NA> -3.405 11.386 17.116  
## 1744 ATOM 1745 CE <NA> LYS B 13 <NA> -3.235 10.212 16.170  
## 1745 ATOM 1746 NZ <NA> LYS B 13 <NA> -3.162 10.603 14.749  
## 1746 ATOM 1747 N <NA> GLY B 14 <NA> -7.355 10.286 19.391  
## 1747 ATOM 1748 CA <NA> GLY B 14 <NA> -8.676 10.152 18.814  
## 1748 ATOM 1749 C <NA> GLY B 14 <NA> -9.757 10.433 19.816  
## 1749 ATOM 1750 O <NA> GLY B 14 <NA> -10.877 10.801 19.472  
## 1750 ATOM 1751 N <NA> THR B 15 <NA> -9.410 10.302 21.082  
## 1751 ATOM 1752 CA <NA> THR B 15 <NA> -10.366 10.540 22.134  
## 1752 ATOM 1753 C <NA> THR B 15 <NA> -10.877 11.961 22.028  
## 1753 ATOM 1754 O <NA> THR B 15 <NA> -12.014 12.241 22.370  
## 1754 ATOM 1755 CB <NA> THR B 15 <NA> -9.720 10.338 23.524  
## 1755 ATOM 1756 OG1 <NA> THR B 15 <NA> -8.724 11.349 23.741  
## 1756 ATOM 1757 CG2 <NA> THR B 15 <NA> -9.080 8.946 23.622  
## 1757 ATOM 1758 N <NA> GLN B 16 <NA> -10.053 12.854 21.509  
## 1758 ATOM 1759 CA <NA> GLN B 16 <NA> -10.451 14.248 21.416  
## 1759 ATOM 1760 C <NA> GLN B 16 <NA> -11.013 14.719 20.070  
## 1760 ATOM 1761 O <NA> GLN B 16 <NA> -11.439 15.874 19.915  
## 1761 ATOM 1762 CB <NA> GLN B 16 <NA> -9.268 15.091 21.845  
## 1762 ATOM 1763 CG <NA> GLN B 16 <NA> -8.827 14.752 23.256  
## 1763 ATOM 1764 CD <NA> GLN B 16 <NA> -9.900 15.051 24.301  
## 1764 ATOM 1765 OE1 <NA> GLN B 16 <NA> -10.772 15.882 24.094  
## 1765 ATOM 1766 NE2 <NA> GLN B 16 <NA> -9.821 14.376 25.434  
## 1766 ATOM 1767 N <NA> ALA B 17 <NA> -11.080 13.795 19.122  
## 1767 ATOM 1768 CA <NA> ALA B 17 <NA> -11.564 14.091 17.787  
## 1768 ATOM 1769 C <NA> ALA B 17 <NA> -13.053 14.404 17.717  
## 1769 ATOM 1770 O <NA> ALA B 17 <NA> -13.439 15.432 17.165  
## 1770 ATOM 1771 CB <NA> ALA B 17 <NA> -11.212 12.967 16.854  
## 1771 ATOM 1772 N <NA> GLN B 18 <NA> -13.891 13.543 18.287  
## 1772 ATOM 1773 CA <NA> GLN B 18 <NA> -15.335 13.777 18.253  
## 1773 ATOM 1774 C <NA> GLN B 18 <NA> -15.651 15.127 18.824  
## 1774 ATOM 1775 O <NA> GLN B 18 <NA> -16.563 15.801 18.372  
## 1775 ATOM 1776 CB <NA> GLN B 18 <NA> -16.085 12.718 19.045  
## 1776 ATOM 1777 CG <NA> GLN B 18 <NA> -17.164 12.016 18.241  
## 1777 ATOM 1778 CD <NA> GLN B 18 <NA> -17.983 11.060 19.080  
## 1778 ATOM 1779 OE1 <NA> GLN B 18 <NA> -17.913 9.833 18.898  
## 1779 ATOM 1780 NE2 <NA> GLN B 18 <NA> -18.780 11.614 20.007  
## 1780 ATOM 1781 N <NA> PHE B 19 <NA> -14.882 15.515 19.827  
## 1781 ATOM 1782 CA <NA> PHE B 19 <NA> -15.058 16.799 20.475  
## 1782 ATOM 1783 C <NA> PHE B 19 <NA> -14.794 17.951 19.517  
## 1783 ATOM 1784 O <NA> PHE B 19 <NA> -15.551 18.926 19.471  
## 1784 ATOM 1785 CB <NA> PHE B 19 <NA> -14.128 16.887 21.683  
## 1785 ATOM 1786 CG <NA> PHE B 19 <NA> -14.003 18.267 22.245  
## 1786 ATOM 1787 CD1 <NA> PHE B 19 <NA> -15.122 18.944 22.706  
## 1787 ATOM 1788 CD2 <NA> PHE B 19 <NA> -12.774 18.914 22.252  
## 1788 ATOM 1789 CE1 <NA> PHE B 19 <NA> -15.013 20.244 23.154  
## 1789 ATOM 1790 CE2 <NA> PHE B 19 <NA> -12.659 20.208 22.697  
## 1790 ATOM 1791 CZ <NA> PHE B 19 <NA> -13.767 20.877 23.145  
## 1791 ATOM 1792 N <NA> ILE B 20 <NA> -13.707 17.827 18.764  
## 1792 ATOM 1793 CA <NA> ILE B 20 <NA> -13.299 18.839 17.810  
## 1793 ATOM 1794 C <NA> ILE B 20 <NA> -14.272 18.953 16.653  
## 1794 ATOM 1795 O <NA> ILE B 20 <NA> -14.579 20.047 16.212  
## 1795 ATOM 1796 CB <NA> ILE B 20 <NA> -11.877 18.555 17.313  
## 1796 ATOM 1797 CG1 <NA> ILE B 20 <NA> -10.906 18.699 18.486  
## 1797 ATOM 1798 CG2 <NA> ILE B 20 <NA> -11.502 19.508 16.201  
## 1798 ATOM 1799 CD1 <NA> ILE B 20 <NA> -9.545 18.188 18.205  
## 1799 ATOM 1800 N <NA> MET B 21 <NA> -14.751 17.820 16.163  
## 1800 ATOM 1801 CA <NA> MET B 21 <NA> -15.724 17.786 15.068  
## 1801 ATOM 1802 C <NA> MET B 21 <NA> -17.035 18.492 15.480  
## 1802 ATOM 1803 O <NA> MET B 21 <NA> -17.568 19.365 14.770  
## 1803 ATOM 1804 CB <NA> MET B 21 <NA> -16.037 16.326 14.689  
## 1804 ATOM 1805 CG <NA> MET B 21 <NA> -14.889 15.553 14.076  
## 1805 ATOM 1806 SD <NA> MET B 21 <NA> -15.453 14.048 13.286  
## 1806 ATOM 1807 CE <NA> MET B 21 <NA> -14.887 12.835 14.273  
## 1807 ATOM 1808 N <NA> GLU B 22 <NA> -17.505 18.151 16.669  
## 1808 ATOM 1809 CA <NA> GLU B 22 <NA> -18.740 18.694 17.202  
## 1809 ATOM 1810 C <NA> GLU B 22 <NA> -18.668 20.168 17.583  
## 1810 ATOM 1811 O <NA> GLU B 22 <NA> -19.679 20.872 17.596  
## 1811 ATOM 1812 CB <NA> GLU B 22 <NA> -19.182 17.857 18.400  
## 1812 ATOM 1813 CG <NA> GLU B 22 <NA> -20.681 17.900 18.670  
## 1813 ATOM 1814 CD <NA> GLU B 22 <NA> -21.137 16.868 19.687  
## 1814 ATOM 1815 OE1 <NA> GLU B 22 <NA> -20.662 15.703 19.632  
## 1815 ATOM 1816 OE2 <NA> GLU B 22 <NA> -21.988 17.226 20.530  
## 1816 ATOM 1817 N <NA> LYS B 23 <NA> -17.478 20.637 17.917  
## 1817 ATOM 1818 CA <NA> LYS B 23 <NA> -17.341 22.028 18.285  
## 1818 ATOM 1819 C <NA> LYS B 23 <NA> -17.293 22.929 17.057  
## 1819 ATOM 1820 O <NA> LYS B 23 <NA> -17.964 23.970 17.011  
## 1820 ATOM 1821 CB <NA> LYS B 23 <NA> -16.095 22.228 19.156  
## 1821 ATOM 1822 CG <NA> LYS B 23 <NA> -15.797 23.691 19.527  
## 1822 ATOM 1823 CD <NA> LYS B 23 <NA> -15.409 23.857 21.006  
## 1823 ATOM 1824 CE <NA> LYS B 23 <NA> -14.647 25.170 21.285  
## 1824 ATOM 1825 NZ <NA> LYS B 23 <NA> -15.436 26.419 21.067  
## 1825 ATOM 1826 N <NA> TYR B 24 <NA> -16.558 22.473 16.041  
## 1826 ATOM 1827 CA <NA> TYR B 24 <NA> -16.334 23.233 14.814  
## 1827 ATOM 1828 C <NA> TYR B 24 <NA> -17.099 22.880 13.557  
## 1828 ATOM 1829 O <NA> TYR B 24 <NA> -17.058 23.634 12.595  
## 1829 ATOM 1830 CB <NA> TYR B 24 <NA> -14.834 23.275 14.524  
## 1830 ATOM 1831 CG <NA> TYR B 24 <NA> -14.074 23.839 15.704  
## 1831 ATOM 1832 CD1 <NA> TYR B 24 <NA> -13.965 25.221 15.893  
## 1832 ATOM 1833 CD2 <NA> TYR B 24 <NA> -13.544 22.994 16.683  
## 1833 ATOM 1834 CE1 <NA> TYR B 24 <NA> -13.358 25.740 17.023  
## 1834 ATOM 1835 CE2 <NA> TYR B 24 <NA> -12.941 23.509 17.815  
## 1835 ATOM 1836 CZ <NA> TYR B 24 <NA> -12.853 24.878 17.972  
## 1836 ATOM 1837 OH <NA> TYR B 24 <NA> -12.267 25.394 19.089  
## 1837 ATOM 1838 N <NA> GLY B 25 <NA> -17.793 21.753 13.537  
## 1838 ATOM 1839 CA <NA> GLY B 25 <NA> -18.534 21.407 12.343  
## 1839 ATOM 1840 C <NA> GLY B 25 <NA> -17.610 21.105 11.187  
## 1840 ATOM 1841 O <NA> GLY B 25 <NA> -17.829 21.564 10.062  
## 1841 ATOM 1842 N <NA> ILE B 26 <NA> -16.621 20.256 11.455  
## 1842 ATOM 1843 CA <NA> ILE B 26 <NA> -15.633 19.865 10.460  
## 1843 ATOM 1844 C <NA> ILE B 26 <NA> -15.463 18.344 10.475  
## 1844 ATOM 1845 O <NA> ILE B 26 <NA> -15.766 17.684 11.473  
## 1845 ATOM 1846 CB <NA> ILE B 26 <NA> -14.289 20.550 10.773  
## 1846 ATOM 1847 CG1 <NA> ILE B 26 <NA> -13.742 20.064 12.128  
## 1847 ATOM 1848 CG2 <NA> ILE B 26 <NA> -14.484 22.046 10.837  
## 1848 ATOM 1849 CD1 <NA> ILE B 26 <NA> -12.419 20.664 12.549  
## 1849 ATOM 1850 N <NA> PRO B 27 <NA> -15.113 17.746 9.327  
## 1850 ATOM 1851 CA <NA> PRO B 27 <NA> -14.943 16.290 9.350  
## 1851 ATOM 1852 C <NA> PRO B 27 <NA> -13.486 15.865 9.620  
## 1852 ATOM 1853 O <NA> PRO B 27 <NA> -12.554 16.657 9.440  
## 1853 ATOM 1854 CB <NA> PRO B 27 <NA> -15.399 15.897 7.957  
## 1854 ATOM 1855 CG <NA> PRO B 27 <NA> -14.957 17.065 7.130  
## 1855 ATOM 1856 CD <NA> PRO B 27 <NA> -15.336 18.234 7.952  
## 1856 ATOM 1857 N <NA> GLN B 28 <NA> -13.303 14.611 10.029  
## 1857 ATOM 1858 CA <NA> GLN B 28 <NA> -11.992 14.016 10.320  
## 1858 ATOM 1859 C <NA> GLN B 28 <NA> -11.477 13.306 9.078  
## 1859 ATOM 1860 O <NA> GLN B 28 <NA> -12.135 12.427 8.528  
## 1860 ATOM 1861 CB <NA> GLN B 28 <NA> -12.119 13.009 11.458  
## 1861 ATOM 1862 CG <NA> GLN B 28 <NA> -10.858 12.231 11.791  
## 1862 ATOM 1863 CD <NA> GLN B 28 <NA> -11.073 11.278 12.959  
## 1863 ATOM 1864 OE1 <NA> GLN B 28 <NA> -12.194 10.847 13.230  
## 1864 ATOM 1865 NE2 <NA> GLN B 28 <NA> -10.003 10.960 13.666  
## 1865 ATOM 1866 N <NA> ILE B 29 <NA> -10.240 13.598 8.717  
## 1866 ATOM 1867 CA <NA> ILE B 29 <NA> -9.644 13.060 7.508  
## 1867 ATOM 1868 C <NA> ILE B 29 <NA> -8.372 12.297 7.778  
## 1868 ATOM 1869 O <NA> ILE B 29 <NA> -7.469 12.785 8.439  
## 1869 ATOM 1870 CB <NA> ILE B 29 <NA> -9.241 14.223 6.581  
## 1870 ATOM 1871 CG1 <NA> ILE B 29 <NA> -10.447 15.092 6.243  
## 1871 ATOM 1872 CG2 <NA> ILE B 29 <NA> -8.522 13.706 5.334  
## 1872 ATOM 1873 CD1 <NA> ILE B 29 <NA> -10.044 16.340 5.533  
## 1873 ATOM 1874 N <NA> SER B 30 <NA> -8.285 11.104 7.235  
## 1874 ATOM 1875 CA <NA> SER B 30 <NA> -7.089 10.326 7.370  
## 1875 ATOM 1876 C <NA> SER B 30 <NA> -6.764 9.923 5.939  
## 1876 ATOM 1877 O <NA> SER B 30 <NA> -7.655 9.736 5.114  
## 1877 ATOM 1878 CB <NA> SER B 30 <NA> -7.328 9.128 8.261  
## 1878 ATOM 1879 OG <NA> SER B 30 <NA> -8.471 8.458 7.825  
## 1879 ATOM 1880 N <NA> THR B 31 <NA> -5.482 9.848 5.626  
## 1880 ATOM 1881 CA <NA> THR B 31 <NA> -5.072 9.510 4.288  
## 1881 ATOM 1882 C <NA> THR B 31 <NA> -5.409 8.072 3.943  
## 1882 ATOM 1883 O <NA> THR B 31 <NA> -5.708 7.773 2.785  
## 1883 ATOM 1884 CB <NA> THR B 31 <NA> -3.588 9.828 4.089  
## 1884 ATOM 1885 OG1 <NA> THR B 31 <NA> -2.806 9.015 4.962  
## 1885 ATOM 1886 CG2 <NA> THR B 31 <NA> -3.343 11.300 4.429  
## 1886 ATOM 1887 N <NA> GLY B 32 <NA> -5.390 7.195 4.944  
## 1887 ATOM 1888 CA <NA> GLY B 32 <NA> -5.734 5.807 4.719  
## 1888 ATOM 1889 C <NA> GLY B 32 <NA> -7.152 5.672 4.176  
## 1889 ATOM 1890 O <NA> GLY B 32 <NA> -7.373 5.000 3.178  
## 1890 ATOM 1891 N <NA> ASP B 33 <NA> -8.118 6.320 4.819  
## 1891 ATOM 1892 CA <NA> ASP B 33 <NA> -9.514 6.261 4.370  
## 1892 ATOM 1893 C <NA> ASP B 33 <NA> -9.589 6.844 2.990  
## 1893 ATOM 1894 O <NA> ASP B 33 <NA> -10.107 6.224 2.066  
## 1894 ATOM 1895 CB <NA> ASP B 33 <NA> -10.440 7.083 5.286  
## 1895 ATOM 1896 CG <NA> ASP B 33 <NA> -10.843 6.338 6.557  
## 1896 ATOM 1897 OD1 <NA> ASP B 33 <NA> -10.682 5.093 6.627  
## 1897 ATOM 1898 OD2 <NA> ASP B 33 <NA> -11.331 7.013 7.492  
## 1898 ATOM 1899 N <NA> MET B 34 <NA> -9.065 8.061 2.901  
## 1899 ATOM 1900 CA <NA> MET B 34 <NA> -8.983 8.876 1.693  
## 1900 ATOM 1901 C <NA> MET B 34 <NA> -8.526 8.086 0.474  
## 1901 ATOM 1902 O <NA> MET B 34 <NA> -9.004 8.312 -0.634  
## 1902 ATOM 1903 CB <NA> MET B 34 <NA> -8.011 10.013 1.956  
## 1903 ATOM 1904 CG <NA> MET B 34 <NA> -8.319 11.265 1.231  
## 1904 ATOM 1905 SD <NA> MET B 34 <NA> -7.091 12.418 1.689  
## 1905 ATOM 1906 CE <NA> MET B 34 <NA> -5.596 11.496 1.118  
## 1906 ATOM 1907 N <NA> LEU B 35 <NA> -7.565 7.194 0.683  
## 1907 ATOM 1908 CA <NA> LEU B 35 <NA> -7.060 6.339 -0.377  
## 1908 ATOM 1909 C <NA> LEU B 35 <NA> -8.094 5.256 -0.661  
## 1909 ATOM 1910 O <NA> LEU B 35 <NA> -8.500 5.081 -1.803  
## 1910 ATOM 1911 CB <NA> LEU B 35 <NA> -5.725 5.707 0.023  
## 1911 ATOM 1912 CG <NA> LEU B 35 <NA> -4.532 6.663 0.026  
## 1912 ATOM 1913 CD1 <NA> LEU B 35 <NA> -3.457 6.157 0.974  
## 1913 ATOM 1914 CD2 <NA> LEU B 35 <NA> -3.995 6.821 -1.386  
## 1914 ATOM 1915 N <NA> ARG B 36 <NA> -8.546 4.543 0.364  
## 1915 ATOM 1916 CA <NA> ARG B 36 <NA> -9.551 3.509 0.151  
## 1916 ATOM 1917 C <NA> ARG B 36 <NA> -10.771 4.045 -0.594  
## 1917 ATOM 1918 O <NA> ARG B 36 <NA> -11.248 3.428 -1.534  
## 1918 ATOM 1919 CB <NA> ARG B 36 <NA> -9.950 2.865 1.471  
## 1919 ATOM 1920 CG <NA> ARG B 36 <NA> -8.889 1.894 1.948  
## 1920 ATOM 1921 CD <NA> ARG B 36 <NA> -9.309 1.142 3.188  
## 1921 ATOM 1922 NE <NA> ARG B 36 <NA> -9.185 1.944 4.398  
## 1922 ATOM 1923 CZ <NA> ARG B 36 <NA> -8.033 2.206 5.011  
## 1923 ATOM 1924 NH1 <NA> ARG B 36 <NA> -6.887 1.743 4.530  
## 1924 ATOM 1925 NH2 <NA> ARG B 36 <NA> -8.027 2.945 6.109  
## 1925 ATOM 1926 N <NA> ALA B 37 <NA> -11.213 5.237 -0.248  
## 1926 ATOM 1927 CA <NA> ALA B 37 <NA> -12.362 5.810 -0.913  
## 1927 ATOM 1928 C <NA> ALA B 37 <NA> -12.139 6.238 -2.376  
## 1928 ATOM 1929 O <NA> ALA B 37 <NA> -13.004 6.008 -3.219  
## 1929 ATOM 1930 CB <NA> ALA B 37 <NA> -12.906 6.971 -0.102  
## 1930 ATOM 1931 N <NA> ALA B 38 <NA> -11.007 6.867 -2.685  
## 1931 ATOM 1932 CA <NA> ALA B 38 <NA> -10.726 7.324 -4.059  
## 1932 ATOM 1933 C <NA> ALA B 38 <NA> -10.621 6.214 -5.111  
## 1933 ATOM 1934 O <NA> ALA B 38 <NA> -10.937 6.431 -6.282  
## 1934 ATOM 1935 CB <NA> ALA B 38 <NA> -9.471 8.179 -4.083  
## 1935 ATOM 1936 N <NA> VAL B 39 <NA> -10.110 5.057 -4.695  
## 1936 ATOM 1937 CA <NA> VAL B 39 <NA> -9.953 3.894 -5.562  
## 1937 ATOM 1938 C <NA> VAL B 39 <NA> -11.343 3.386 -5.891  
## 1938 ATOM 1939 O <NA> VAL B 39 <NA> -11.656 3.111 -7.049  
## 1939 ATOM 1940 CB <NA> VAL B 39 <NA> -9.165 2.774 -4.855  
## 1940 ATOM 1941 CG1 <NA> VAL B 39 <NA> -9.307 1.480 -5.615  
## 1941 ATOM 1942 CG2 <NA> VAL B 39 <NA> -7.692 3.156 -4.740  
## 1942 ATOM 1943 N <NA> LYS B 40 <NA> -12.165 3.280 -4.850  
## 1943 ATOM 1944 CA <NA> LYS B 40 <NA> -13.553 2.826 -4.944  
## 1944 ATOM 1945 C <NA> LYS B 40 <NA> -14.255 3.598 -6.057  
## 1945 ATOM 1946 O <NA> LYS B 40 <NA> -14.612 3.020 -7.085  
## 1946 ATOM 1947 CB <NA> LYS B 40 <NA> -14.246 3.016 -3.575  
## 1947 ATOM 1948 CG <NA> LYS B 40 <NA> -15.790 3.010 -3.531  
## 1948 ATOM 1949 CD <NA> LYS B 40 <NA> -16.382 4.444 -3.390  
## 1949 ATOM 1950 CE <NA> LYS B 40 <NA> -15.990 5.152 -2.078  
## 1950 ATOM 1951 NZ <NA> LYS B 40 <NA> -16.312 6.618 -2.063  
## 1951 ATOM 1952 N <NA> SER B 41 <NA> -14.442 4.900 -5.864  
## 1952 ATOM 1953 CA <NA> SER B 41 <NA> -15.073 5.708 -6.896  
## 1953 ATOM 1954 C <NA> SER B 41 <NA> -13.968 6.151 -7.844  
## 1954 ATOM 1955 O <NA> SER B 41 <NA> -13.354 7.217 -7.681  
## 1955 ATOM 1956 CB <NA> SER B 41 <NA> -15.863 6.896 -6.313  
## 1956 ATOM 1957 OG <NA> SER B 41 <NA> -15.141 7.591 -5.312  
## 1957 ATOM 1958 N <NA> GLY B 42 <NA> -13.665 5.252 -8.775  
## 1958 ATOM 1959 CA <NA> GLY B 42 <NA> -12.648 5.493 -9.771  
## 1959 ATOM 1960 C <NA> GLY B 42 <NA> -12.627 6.899 -10.342  
## 1960 ATOM 1961 O <NA> GLY B 42 <NA> -13.522 7.326 -11.072  
## 1961 ATOM 1962 N <NA> SER B 43 <NA> -11.627 7.647 -9.908  
## 1962 ATOM 1963 CA <NA> SER B 43 <NA> -11.382 8.995 -10.373  
## 1963 ATOM 1964 C <NA> SER B 43 <NA> -9.971 8.841 -10.949  
## 1964 ATOM 1965 O <NA> SER B 43 <NA> -9.360 7.782 -10.797  
## 1965 ATOM 1966 CB <NA> SER B 43 <NA> -11.416 9.975 -9.190  
## 1966 ATOM 1967 OG <NA> SER B 43 <NA> -10.834 9.424 -8.013  
## 1967 ATOM 1968 N <NA> GLU B 44 <NA> -9.461 9.845 -11.648  
## 1968 ATOM 1969 CA <NA> GLU B 44 <NA> -8.109 9.755 -12.206  
## 1969 ATOM 1970 C <NA> GLU B 44 <NA> -7.133 9.267 -11.115  
## 1970 ATOM 1971 O <NA> GLU B 44 <NA> -6.630 8.145 -11.180  
## 1971 ATOM 1972 CB <NA> GLU B 44 <NA> -7.684 11.130 -12.750  
## 1972 ATOM 1973 CG <NA> GLU B 44 <NA> -6.251 11.224 -13.283  
## 1973 ATOM 1974 CD <NA> GLU B 44 <NA> -6.028 10.449 -14.574  
## 1974 ATOM 1975 OE1 <NA> GLU B 44 <NA> -6.901 10.499 -15.474  
## 1975 ATOM 1976 OE2 <NA> GLU B 44 <NA> -4.964 9.798 -14.688  
## 1976 ATOM 1977 N <NA> LEU B 45 <NA> -6.956 10.084 -10.076  
## 1977 ATOM 1978 CA <NA> LEU B 45 <NA> -6.074 9.781 -8.948  
## 1978 ATOM 1979 C <NA> LEU B 45 <NA> -6.317 8.405 -8.325  
## 1979 ATOM 1980 O <NA> LEU B 45 <NA> -5.384 7.615 -8.193  
## 1980 ATOM 1981 CB <NA> LEU B 45 <NA> -6.208 10.869 -7.886  
## 1981 ATOM 1982 CG <NA> LEU B 45 <NA> -5.492 12.207 -8.112  
## 1982 ATOM 1983 CD1 <NA> LEU B 45 <NA> -4.947 12.311 -9.522  
## 1983 ATOM 1984 CD2 <NA> LEU B 45 <NA> -6.423 13.377 -7.793  
## 1984 ATOM 1985 N <NA> GLY B 46 <NA> -7.568 8.113 -7.973  
## 1985 ATOM 1986 CA <NA> GLY B 46 <NA> -7.911 6.829 -7.381  
## 1986 ATOM 1987 C <NA> GLY B 46 <NA> -7.534 5.651 -8.258  
## 1987 ATOM 1988 O <NA> GLY B 46 <NA> -7.369 4.521 -7.770  
## 1988 ATOM 1989 N <NA> LYS B 47 <NA> -7.469 5.905 -9.563  
## 1989 ATOM 1990 CA <NA> LYS B 47 <NA> -7.080 4.898 -10.537  
## 1990 ATOM 1991 C <NA> LYS B 47 <NA> -5.564 4.800 -10.461  
## 1991 ATOM 1992 O <NA> LYS B 47 <NA> -5.003 3.720 -10.579  
## 1992 ATOM 1993 CB <NA> LYS B 47 <NA> -7.506 5.293 -11.954  
## 1993 ATOM 1994 CG <NA> LYS B 47 <NA> -9.007 5.185 -12.271  
## 1994 ATOM 1995 CD <NA> LYS B 47 <NA> -9.456 3.761 -12.645  
## 1995 ATOM 1996 CE <NA> LYS B 47 <NA> -9.798 2.894 -11.420  
## 1996 ATOM 1997 NZ <NA> LYS B 47 <NA> -10.388 1.565 -11.797  
## 1997 ATOM 1998 N <NA> GLN B 48 <NA> -4.892 5.926 -10.270  
## 1998 ATOM 1999 CA <NA> GLN B 48 <NA> -3.447 5.881 -10.147  
## 1999 ATOM 2000 C <NA> GLN B 48 <NA> -3.068 5.193 -8.836  
## 2000 ATOM 2001 O <NA> GLN B 48 <NA> -2.136 4.395 -8.798  
## 2001 ATOM 2002 CB <NA> GLN B 48 <NA> -2.849 7.281 -10.219  
## 2002 ATOM 2003 CG <NA> GLN B 48 <NA> -3.182 7.988 -11.522  
## 2003 ATOM 2004 CD <NA> GLN B 48 <NA> -2.276 9.169 -11.810  
## 2004 ATOM 2005 OE1 <NA> GLN B 48 <NA> -1.261 9.364 -11.145  
## 2005 ATOM 2006 NE2 <NA> GLN B 48 <NA> -2.622 9.946 -12.831  
## 2006 ATOM 2007 N <NA> ALA B 49 <NA> -3.835 5.449 -7.783  
## 2007 ATOM 2008 CA <NA> ALA B 49 <NA> -3.586 4.861 -6.467  
## 2008 ATOM 2009 C <NA> ALA B 49 <NA> -3.800 3.363 -6.466  
## 2009 ATOM 2010 O <NA> ALA B 49 <NA> -2.941 2.614 -6.010  
## 2010 ATOM 2011 CB <NA> ALA B 49 <NA> -4.478 5.504 -5.423  
## 2011 ATOM 2012 N <NA> LYS B 50 <NA> -4.960 2.943 -6.963  
## 2012 ATOM 2013 CA <NA> LYS B 50 <NA> -5.327 1.534 -7.056  
## 2013 ATOM 2014 C <NA> LYS B 50 <NA> -4.260 0.687 -7.758  
## 2014 ATOM 2015 O <NA> LYS B 50 <NA> -4.031 -0.463 -7.383  
## 2015 ATOM 2016 CB <NA> LYS B 50 <NA> -6.643 1.404 -7.811  
## 2016 ATOM 2017 CG <NA> LYS B 50 <NA> -6.999 -0.013 -8.182  
## 2017 ATOM 2018 CD <NA> LYS B 50 <NA> -8.304 -0.066 -8.960  
## 2018 ATOM 2019 CE <NA> LYS B 50 <NA> -8.658 -1.495 -9.412  
## 2019 ATOM 2020 NZ <NA> LYS B 50 <NA> -8.020 -1.934 -10.694  
## 2020 ATOM 2021 N <NA> ASP B 51 <NA> -3.635 1.245 -8.793  
## 2021 ATOM 2022 CA <NA> ASP B 51 <NA> -2.587 0.555 -9.559  
## 2022 ATOM 2023 C <NA> ASP B 51 <NA> -1.335 0.303 -8.746  
## 2023 ATOM 2024 O <NA> ASP B 51 <NA> -0.758 -0.783 -8.786  
## 2024 ATOM 2025 CB <NA> ASP B 51 <NA> -2.190 1.373 -10.791  
## 2025 ATOM 2026 CG <NA> ASP B 51 <NA> -2.885 0.912 -12.057  
## 2026 ATOM 2027 OD1 <NA> ASP B 51 <NA> -3.272 -0.279 -12.133  
## 2027 ATOM 2028 OD2 <NA> ASP B 51 <NA> -3.021 1.743 -12.984  
## 2028 ATOM 2029 N <NA> ILE B 52 <NA> -0.876 1.348 -8.072  
## 2029 ATOM 2030 CA <NA> ILE B 52 <NA> 0.305 1.281 -7.234  
## 2030 ATOM 2031 C <NA> ILE B 52 <NA> 0.116 0.243 -6.133  
## 2031 ATOM 2032 O <NA> ILE B 52 <NA> 0.934 -0.645 -5.970  
## 2032 ATOM 2033 CB <NA> ILE B 52 <NA> 0.594 2.669 -6.663  
## 2033 ATOM 2034 CG1 <NA> ILE B 52 <NA> 1.294 3.511 -7.730  
## 2034 ATOM 2035 CG2 <NA> ILE B 52 <NA> 1.406 2.573 -5.410  
## 2035 ATOM 2036 CD1 <NA> ILE B 52 <NA> 1.619 4.910 -7.286  
## 2036 ATOM 2037 N <NA> MET B 53 <NA> -1.008 0.327 -5.438  
## 2037 ATOM 2038 CA <NA> MET B 53 <NA> -1.344 -0.594 -4.363  
## 2038 ATOM 2039 C <NA> MET B 53 <NA> -1.467 -2.036 -4.839  
## 2039 ATOM 2040 O <NA> MET B 53 <NA> -1.115 -2.986 -4.130  
## 2040 ATOM 2041 CB <NA> MET B 53 <NA> -2.664 -0.160 -3.718  
## 2041 ATOM 2042 CG <NA> MET B 53 <NA> -2.631 1.247 -3.122  
## 2042 ATOM 2043 SD <NA> MET B 53 <NA> -4.043 1.557 -2.039  
## 2043 ATOM 2044 CE <NA> MET B 53 <NA> -4.386 -0.126 -1.411  
## 2044 ATOM 2045 N <NA> ASP B 54 <NA> -2.042 -2.206 -6.018  
## 2045 ATOM 2046 CA <NA> ASP B 54 <NA> -2.188 -3.533 -6.580  
## 2046 ATOM 2047 C <NA> ASP B 54 <NA> -0.820 -4.083 -6.975  
## 2047 ATOM 2048 O <NA> ASP B 54 <NA> -0.621 -5.291 -6.981  
## 2048 ATOM 2049 CB <NA> ASP B 54 <NA> -3.143 -3.516 -7.775  
## 2049 ATOM 2050 CG <NA> ASP B 54 <NA> -4.571 -3.890 -7.386  
## 2050 ATOM 2051 OD1 <NA> ASP B 54 <NA> -4.768 -5.019 -6.872  
## 2051 ATOM 2052 OD2 <NA> ASP B 54 <NA> -5.490 -3.063 -7.592  
## 2052 ATOM 2053 N <NA> ALA B 55 <NA> 0.128 -3.202 -7.293  
## 2053 ATOM 2054 CA <NA> ALA B 55 <NA> 1.483 -3.621 -7.666  
## 2054 ATOM 2055 C <NA> ALA B 55 <NA> 2.376 -3.784 -6.437  
## 2055 ATOM 2056 O <NA> ALA B 55 <NA> 3.583 -4.008 -6.571  
## 2056 ATOM 2057 CB <NA> ALA B 55 <NA> 2.092 -2.610 -8.596  
## 2057 ATOM 2058 N <NA> GLY B 56 <NA> 1.798 -3.593 -5.248  
## 2058 ATOM 2059 CA <NA> GLY B 56 <NA> 2.546 -3.722 -4.008  
## 2059 ATOM 2060 C <NA> GLY B 56 <NA> 3.564 -2.631 -3.761  
## 2060 ATOM 2061 O <NA> GLY B 56 <NA> 4.499 -2.813 -2.973  
## 2061 ATOM 2062 N <NA> LYS B 57 <NA> 3.379 -1.501 -4.436  
## 2062 ATOM 2063 CA <NA> LYS B 57 <NA> 4.262 -0.341 -4.318  
## 2063 ATOM 2064 C <NA> LYS B 57 <NA> 3.633 0.654 -3.347  
## 2064 ATOM 2065 O <NA> LYS B 57 <NA> 2.416 0.653 -3.132  
## 2065 ATOM 2066 CB <NA> LYS B 57 <NA> 4.412 0.365 -5.665  
## 2066 ATOM 2067 CG <NA> LYS B 57 <NA> 5.067 -0.422 -6.768  
## 2067 ATOM 2068 CD <NA> LYS B 57 <NA> 4.753 0.232 -8.101  
## 2068 ATOM 2069 CE <NA> LYS B 57 <NA> 5.128 -0.661 -9.275  
## 2069 ATOM 2070 NZ <NA> LYS B 57 <NA> 4.610 -0.127 -10.580  
## 2070 ATOM 2071 N <NA> LEU B 58 <NA> 4.452 1.548 -2.816  
## 2071 ATOM 2072 CA <NA> LEU B 58 <NA> 3.975 2.548 -1.883  
## 2072 ATOM 2073 C <NA> LEU B 58 <NA> 3.458 3.731 -2.676  
## 2073 ATOM 2074 O <NA> LEU B 58 <NA> 4.012 4.079 -3.724  
## 2074 ATOM 2075 CB <NA> LEU B 58 <NA> 5.112 2.963 -0.949  
## 2075 ATOM 2076 CG <NA> LEU B 58 <NA> 4.809 3.919 0.204  
## 2076 ATOM 2077 CD1 <NA> LEU B 58 <NA> 5.637 3.496 1.395  
## 2077 ATOM 2078 CD2 <NA> LEU B 58 <NA> 5.117 5.373 -0.176  
## 2078 ATOM 2079 N <NA> VAL B 59 <NA> 2.393 4.347 -2.184  
## 2079 ATOM 2080 CA <NA> VAL B 59 <NA> 1.834 5.484 -2.886  
## 2080 ATOM 2081 C <NA> VAL B 59 <NA> 2.748 6.683 -2.735  
## 2081 ATOM 2082 O <NA> VAL B 59 <NA> 3.202 7.013 -1.643  
## 2082 ATOM 2083 CB <NA> VAL B 59 <NA> 0.416 5.837 -2.416  
## 2083 ATOM 2084 CG1 <NA> VAL B 59 <NA> -0.266 6.725 -3.463  
## 2084 ATOM 2085 CG2 <NA> VAL B 59 <NA> -0.391 4.563 -2.194  
## 2085 ATOM 2086 N <NA> THR B 60 <NA> 3.034 7.308 -3.864  
## 2086 ATOM 2087 CA <NA> THR B 60 <NA> 3.906 8.456 -3.920  
## 2087 ATOM 2088 C <NA> THR B 60 <NA> 3.324 9.660 -3.169  
## 2088 ATOM 2089 O <NA> THR B 60 <NA> 2.127 9.910 -3.218  
## 2089 ATOM 2090 CB <NA> THR B 60 <NA> 4.201 8.792 -5.410  
## 2090 ATOM 2091 OG1 <NA> THR B 60 <NA> 5.082 9.912 -5.491  
## 2091 ATOM 2092 CG2 <NA> THR B 60 <NA> 2.924 9.125 -6.162  
## 2092 ATOM 2093 N <NA> ASP B 61 <NA> 4.174 10.409 -2.477  
## 2093 ATOM 2094 CA <NA> ASP B 61 <NA> 3.733 11.597 -1.742  
## 2094 ATOM 2095 C <NA> ASP B 61 <NA> 3.046 12.534 -2.694  
## 2095 ATOM 2096 O <NA> ASP B 61 <NA> 2.308 13.429 -2.298  
## 2096 ATOM 2097 CB <NA> ASP B 61 <NA> 4.920 12.372 -1.176  
## 2097 ATOM 2098 CG <NA> ASP B 61 <NA> 5.537 11.720 0.038  
## 2098 ATOM 2099 OD1 <NA> ASP B 61 <NA> 4.992 10.700 0.533  
## 2099 ATOM 2100 OD2 <NA> ASP B 61 <NA> 6.587 12.250 0.483  
## 2100 ATOM 2101 N <NA> GLU B 62 <NA> 3.382 12.378 -3.958  
## 2101 ATOM 2102 CA <NA> GLU B 62 <NA> 2.833 13.210 -4.996  
## 2102 ATOM 2103 C <NA> GLU B 62 <NA> 1.333 12.921 -5.155  
## 2103 ATOM 2104 O <NA> GLU B 62 <NA> 0.522 13.850 -5.241  
## 2104 ATOM 2105 CB <NA> GLU B 62 <NA> 3.638 12.976 -6.281  
## 2105 ATOM 2106 CG <NA> GLU B 62 <NA> 5.057 13.655 -6.324  
## 2106 ATOM 2107 CD <NA> GLU B 62 <NA> 6.097 13.176 -5.265  
## 2107 ATOM 2108 OE1 <NA> GLU B 62 <NA> 6.562 12.014 -5.328  
## 2108 ATOM 2109 OE2 <NA> GLU B 62 <NA> 6.506 14.003 -4.407  
## 2109 ATOM 2110 N <NA> LEU B 63 <NA> 0.957 11.642 -5.110  
## 2110 ATOM 2111 CA <NA> LEU B 63 <NA> -0.448 11.264 -5.235  
## 2111 ATOM 2112 C <NA> LEU B 63 <NA> -1.196 11.681 -3.994  
## 2112 ATOM 2113 O <NA> LEU B 63 <NA> -2.202 12.369 -4.087  
## 2113 ATOM 2114 CB <NA> LEU B 63 <NA> -0.627 9.760 -5.448  
## 2114 ATOM 2115 CG <NA> LEU B 63 <NA> -1.087 9.349 -6.851  
## 2115 ATOM 2116 CD1 <NA> LEU B 63 <NA> -1.572 7.923 -6.788  
## 2116 ATOM 2117 CD2 <NA> LEU B 63 <NA> -2.215 10.256 -7.348  
## 2117 ATOM 2118 N <NA> VAL B 64 <NA> -0.686 11.295 -2.831  
## 2118 ATOM 2119 CA <NA> VAL B 64 <NA> -1.322 11.653 -1.567  
## 2119 ATOM 2120 C <NA> VAL B 64 <NA> -1.645 13.146 -1.437  
## 2120 ATOM 2121 O <NA> VAL B 64 <NA> -2.765 13.489 -1.068  
## 2121 ATOM 2122 CB <NA> VAL B 64 <NA> -0.511 11.144 -0.350  
## 2122 ATOM 2123 CG1 <NA> VAL B 64 <NA> -1.108 11.645 0.948  
## 2123 ATOM 2124 CG2 <NA> VAL B 64 <NA> -0.525 9.639 -0.344  
## 2124 ATOM 2125 N <NA> ILE B 65 <NA> -0.718 14.038 -1.779  
## 2125 ATOM 2126 CA <NA> ILE B 65 <NA> -1.009 15.479 -1.670  
## 2126 ATOM 2127 C <NA> ILE B 65 <NA> -2.118 15.933 -2.625  
## 2127 ATOM 2128 O <NA> ILE B 65 <NA> -2.865 16.865 -2.307  
## 2128 ATOM 2129 CB <NA> ILE B 65 <NA> 0.244 16.375 -1.867  
## 2129 ATOM 2130 CG1 <NA> ILE B 65 <NA> 1.184 16.235 -0.669  
## 2130 ATOM 2131 CG2 <NA> ILE B 65 <NA> -0.154 17.822 -1.916  
## 2131 ATOM 2132 CD1 <NA> ILE B 65 <NA> 0.573 16.710 0.629  
## 2132 ATOM 2133 N <NA> ALA B 66 <NA> -2.235 15.271 -3.779  
## 2133 ATOM 2134 CA <NA> ALA B 66 <NA> -3.262 15.601 -4.769  
## 2134 ATOM 2135 C <NA> ALA B 66 <NA> -4.640 15.135 -4.292  
## 2135 ATOM 2136 O <NA> ALA B 66 <NA> -5.643 15.827 -4.512  
## 2136 ATOM 2137 CB <NA> ALA B 66 <NA> -2.916 14.978 -6.120  
## 2137 ATOM 2138 N <NA> LEU B 67 <NA> -4.671 13.961 -3.645  
## 2138 ATOM 2139 CA <NA> LEU B 67 <NA> -5.888 13.373 -3.073  
## 2139 ATOM 2140 C <NA> LEU B 67 <NA> -6.370 14.206 -1.900  
## 2140 ATOM 2141 O <NA> LEU B 67 <NA> -7.573 14.296 -1.681  
## 2141 ATOM 2142 CB <NA> LEU B 67 <NA> -5.654 11.940 -2.599  
## 2142 ATOM 2143 CG <NA> LEU B 67 <NA> -5.715 10.858 -3.673  
## 2143 ATOM 2144 CD1 <NA> LEU B 67 <NA> -5.290 9.504 -3.127  
## 2144 ATOM 2145 CD2 <NA> LEU B 67 <NA> -7.124 10.803 -4.200  
## 2145 ATOM 2146 N <NA> VAL B 68 <NA> -5.442 14.818 -1.155  
## 2146 ATOM 2147 CA <NA> VAL B 68 <NA> -5.794 15.672 -0.013  
## 2147 ATOM 2148 C <NA> VAL B 68 <NA> -6.369 16.960 -0.536  
## 2148 ATOM 2149 O <NA> VAL B 68 <NA> -7.414 17.416 -0.082  
## 2149 ATOM 2150 CB <NA> VAL B 68 <NA> -4.582 16.053 0.859  
## 2150 ATOM 2151 CG1 <NA> VAL B 68 <NA> -4.973 17.146 1.840  
## 2151 ATOM 2152 CG2 <NA> VAL B 68 <NA> -4.088 14.868 1.624  
## 2152 ATOM 2153 N <NA> LYS B 69 <NA> -5.657 17.571 -1.470  
## 2153 ATOM 2154 CA <NA> LYS B 69 <NA> -6.115 18.811 -2.067  
## 2154 ATOM 2155 C <NA> LYS B 69 <NA> -7.467 18.573 -2.731  
## 2155 ATOM 2156 O <NA> LYS B 69 <NA> -8.292 19.477 -2.778  
## 2156 ATOM 2157 CB <NA> LYS B 69 <NA> -5.098 19.352 -3.070  
## 2157 ATOM 2158 CG <NA> LYS B 69 <NA> -5.379 20.782 -3.462  
## 2158 ATOM 2159 CD <NA> LYS B 69 <NA> -4.310 21.355 -4.374  
## 2159 ATOM 2160 CE <NA> LYS B 69 <NA> -4.886 21.779 -5.723  
## 2160 ATOM 2161 NZ <NA> LYS B 69 <NA> -5.393 20.616 -6.521  
## 2161 ATOM 2162 N <NA> GLU B 70 <NA> -7.689 17.358 -3.231  
## 2162 ATOM 2163 CA <NA> GLU B 70 <NA> -8.962 16.980 -3.856  
## 2163 ATOM 2164 C <NA> GLU B 70 <NA> -10.072 16.827 -2.786  
## 2164 ATOM 2165 O <NA> GLU B 70 <NA> -11.178 17.362 -2.938  
## 2165 ATOM 2166 CB <NA> GLU B 70 <NA> -8.798 15.670 -4.630  
## 2166 ATOM 2167 CG <NA> GLU B 70 <NA> -10.082 15.134 -5.261  
## 2167 ATOM 2168 CD <NA> GLU B 70 <NA> -9.966 13.676 -5.726  
## 2168 ATOM 2169 OE1 <NA> GLU B 70 <NA> -9.906 12.760 -4.865  
## 2169 ATOM 2170 OE2 <NA> GLU B 70 <NA> -9.960 13.446 -6.957  
## 2170 ATOM 2171 N <NA> ARG B 71 <NA> -9.763 16.112 -1.703  
## 2171 ATOM 2172 CA <NA> ARG B 71 <NA> -10.700 15.897 -0.606  
## 2172 ATOM 2173 C <NA> ARG B 71 <NA> -11.154 17.187 0.077  
## 2173 ATOM 2174 O <NA> ARG B 71 <NA> -12.352 17.501 0.129  
## 2174 ATOM 2175 CB <NA> ARG B 71 <NA> -10.077 14.993 0.449  
## 2175 ATOM 2176 CG <NA> ARG B 71 <NA> -10.997 14.736 1.627  
## 2176 ATOM 2177 CD <NA> ARG B 71 <NA> -12.259 13.991 1.176  
## 2177 ATOM 2178 NE <NA> ARG B 71 <NA> -13.212 13.792 2.264  
## 2178 ATOM 2179 CZ <NA> ARG B 71 <NA> -14.017 14.735 2.744  
## 2179 ATOM 2180 NH1 <NA> ARG B 71 <NA> -14.021 15.963 2.236  
## 2180 ATOM 2181 NH2 <NA> ARG B 71 <NA> -14.834 14.440 3.738  
## 2181 ATOM 2182 N <NA> ILE B 72 <NA> -10.195 17.951 0.583  
## 2182 ATOM 2183 CA <NA> ILE B 72 <NA> -10.521 19.185 1.279  
## 2183 ATOM 2184 C <NA> ILE B 72 <NA> -11.256 20.164 0.376  
## 2184 ATOM 2185 O <NA> ILE B 72 <NA> -11.613 21.278 0.788  
## 2185 ATOM 2186 CB <NA> ILE B 72 <NA> -9.258 19.852 1.872  
## 2186 ATOM 2187 CG1 <NA> ILE B 72 <NA> -8.292 20.216 0.758  
## 2187 ATOM 2188 CG2 <NA> ILE B 72 <NA> -8.572 18.912 2.843  
## 2188 ATOM 2189 CD1 <NA> ILE B 72 <NA> -7.708 21.570 0.934  
## 2189 ATOM 2190 N <NA> ALA B 73 <NA> -11.467 19.746 -0.866  
## 2190 ATOM 2191 CA <NA> ALA B 73 <NA> -12.154 20.569 -1.860  
## 2191 ATOM 2192 C <NA> ALA B 73 <NA> -13.669 20.420 -1.777  
## 2192 ATOM 2193 O <NA> ALA B 73 <NA> -14.412 21.046 -2.539  
## 2193 ATOM 2194 CB <NA> ALA B 73 <NA> -11.680 20.195 -3.270  
## 2194 ATOM 2195 N <NA> GLN B 74 <NA> -14.142 19.604 -0.851  
## 2195 ATOM 2196 CA <NA> GLN B 74 <NA> -15.558 19.408 -0.778  
## 2196 ATOM 2197 C <NA> GLN B 74 <NA> -16.368 20.319 0.124  
## 2197 ATOM 2198 O <NA> GLN B 74 <NA> -15.845 21.189 0.824  
## 2198 ATOM 2199 CB <NA> GLN B 74 <NA> -15.829 17.946 -0.544  
## 2199 ATOM 2200 CG <NA> GLN B 74 <NA> -14.983 17.131 -1.485  
## 2200 ATOM 2201 CD <NA> GLN B 74 <NA> -15.401 15.696 -1.567  
## 2201 ATOM 2202 OE1 <NA> GLN B 74 <NA> -14.596 14.825 -1.905  
## 2202 ATOM 2203 NE2 <NA> GLN B 74 <NA> -16.679 15.429 -1.292  
## 2203 ATOM 2204 N <NA> GLU B 75 <NA> -17.673 20.200 -0.070  
## 2204 ATOM 2205 CA <NA> GLU B 75 <NA> -18.716 20.927 0.644  
## 2205 ATOM 2206 C <NA> GLU B 75 <NA> -18.541 20.800 2.160  
## 2206 ATOM 2207 O <NA> GLU B 75 <NA> -18.633 21.790 2.901  
## 2207 ATOM 2208 CB <NA> GLU B 75 <NA> -20.086 20.340 0.251  
## 2208 ATOM 2209 CG <NA> GLU B 75 <NA> -20.113 19.428 -1.022  
## 2209 ATOM 2210 CD <NA> GLU B 75 <NA> -19.358 18.072 -0.888  
## 2210 ATOM 2211 OE1 <NA> GLU B 75 <NA> -18.928 17.709 0.231  
## 2211 ATOM 2212 OE2 <NA> GLU B 75 <NA> -19.177 17.370 -1.917  
## 2212 ATOM 2213 N <NA> ASP B 76 <NA> -18.286 19.564 2.599  
## 2213 ATOM 2214 CA <NA> ASP B 76 <NA> -18.104 19.233 4.010  
## 2214 ATOM 2215 C <NA> ASP B 76 <NA> -16.846 19.812 4.633  
## 2215 ATOM 2216 O <NA> ASP B 76 <NA> -16.718 19.832 5.863  
## 2216 ATOM 2217 CB <NA> ASP B 76 <NA> -18.131 17.724 4.225  
## 2217 ATOM 2218 CG <NA> ASP B 76 <NA> -17.114 16.993 3.390  
## 2218 ATOM 2219 OD1 <NA> ASP B 76 <NA> -16.293 17.648 2.720  
## 2219 ATOM 2220 OD2 <NA> ASP B 76 <NA> -17.135 15.744 3.406  
## 2220 ATOM 2221 N <NA> CYS B 77 <NA> -15.890 20.210 3.798  
## 2221 ATOM 2222 CA <NA> CYS B 77 <NA> -14.678 20.810 4.320  
## 2222 ATOM 2223 C <NA> CYS B 77 <NA> -14.781 22.322 4.185  
## 2223 ATOM 2224 O <NA> CYS B 77 <NA> -13.786 23.044 4.264  
## 2224 ATOM 2225 CB <NA> CYS B 77 <NA> -13.429 20.263 3.635  
## 2225 ATOM 2226 SG <NA> CYS B 77 <NA> -13.197 18.509 3.863  
## 2226 ATOM 2227 N <NA> ARG B 78 <NA> -16.007 22.808 4.021  
## 2227 ATOM 2228 CA <NA> ARG B 78 <NA> -16.230 24.240 3.916  
## 2228 ATOM 2229 C <NA> ARG B 78 <NA> -15.810 24.905 5.230  
## 2229 ATOM 2230 O <NA> ARG B 78 <NA> -15.096 25.912 5.210  
## 2230 ATOM 2231 CB <NA> ARG B 78 <NA> -17.701 24.539 3.601  
## 2231 ATOM 2232 CG <NA> ARG B 78 <NA> -17.987 26.019 3.324  
## 2232 ATOM 2233 CD <NA> ARG B 78 <NA> -19.240 26.230 2.457  
## 2233 ATOM 2234 NE <NA> ARG B 78 <NA> -19.037 25.871 1.048  
## 2234 ATOM 2235 CZ <NA> ARG B 78 <NA> -19.349 24.688 0.512  
## 2235 ATOM 2236 NH1 <NA> ARG B 78 <NA> -19.880 23.722 1.260  
## 2236 ATOM 2237 NH2 <NA> ARG B 78 <NA> -19.124 24.465 -0.779  
## 2237 ATOM 2238 N <NA> ASN B 79 <NA> -16.219 24.317 6.362  
## 2238 ATOM 2239 CA <NA> ASN B 79 <NA> -15.882 24.847 7.694  
## 2239 ATOM 2240 C <NA> ASN B 79 <NA> -14.448 24.521 8.088  
## 2240 ATOM 2241 O <NA> ASN B 79 <NA> -13.927 25.035 9.076  
## 2241 ATOM 2242 CB <NA> ASN B 79 <NA> -16.808 24.272 8.767  
## 2242 ATOM 2243 CG <NA> ASN B 79 <NA> -18.212 24.814 8.685  
## 2243 ATOM 2244 OD1 <NA> ASN B 79 <NA> -18.437 25.923 8.211  
## 2244 ATOM 2245 ND2 <NA> ASN B 79 <NA> -19.167 24.043 9.176  
## 2245 ATOM 2246 N <NA> GLY B 80 <NA> -13.842 23.598 7.357  
## 2246 ATOM 2247 CA <NA> GLY B 80 <NA> -12.481 23.217 7.645  
## 2247 ATOM 2248 C <NA> GLY B 80 <NA> -12.362 21.714 7.647  
## 2248 ATOM 2249 O <NA> GLY B 80 <NA> -13.183 21.026 7.057  
## 2249 ATOM 2250 N <NA> PHE B 81 <NA> -11.378 21.198 8.369  
## 2250 ATOM 2251 CA <NA> PHE B 81 <NA> -11.155 19.758 8.429  
## 2251 ATOM 2252 C <NA> PHE B 81 <NA> -10.206 19.372 9.569  
## 2252 ATOM 2253 O <NA> PHE B 81 <NA> -9.482 20.214 10.098  
## 2253 ATOM 2254 CB <NA> PHE B 81 <NA> -10.567 19.302 7.110  
## 2254 ATOM 2255 CG <NA> PHE B 81 <NA> -9.316 20.041 6.710  
## 2255 ATOM 2256 CD1 <NA> PHE B 81 <NA> -8.079 19.689 7.250  
## 2256 ATOM 2257 CD2 <NA> PHE B 81 <NA> -9.375 21.074 5.784  
## 2257 ATOM 2258 CE1 <NA> PHE B 81 <NA> -6.938 20.351 6.878  
## 2258 ATOM 2259 CE2 <NA> PHE B 81 <NA> -8.236 21.743 5.400  
## 2259 ATOM 2260 CZ <NA> PHE B 81 <NA> -7.012 21.387 5.947  
## 2260 ATOM 2261 N <NA> LEU B 82 <NA> -10.231 18.108 9.965  
## 2261 ATOM 2262 CA <NA> LEU B 82 <NA> -9.339 17.646 11.008  
## 2262 ATOM 2263 C <NA> LEU B 82 <NA> -8.566 16.532 10.336  
## 2263 ATOM 2264 O <NA> LEU B 82 <NA> -9.111 15.475 10.063  
## 2264 ATOM 2265 CB <NA> LEU B 82 <NA> -10.113 17.133 12.224  
## 2265 ATOM 2266 CG <NA> LEU B 82 <NA> -9.366 16.307 13.277  
## 2266 ATOM 2267 CD1 <NA> LEU B 82 <NA> -8.508 17.194 14.123  
## 2267 ATOM 2268 CD2 <NA> LEU B 82 <NA> -10.373 15.558 14.158  
## 2268 ATOM 2269 N <NA> LEU B 83 <NA> -7.326 16.840 9.965  
## 2269 ATOM 2270 CA <NA> LEU B 83 <NA> -6.422 15.905 9.306  
## 2270 ATOM 2271 C <NA> LEU B 83 <NA> -5.675 15.151 10.390  
## 2271 ATOM 2272 O <NA> LEU B 83 <NA> -4.863 15.689 11.147  
## 2272 ATOM 2273 CB <NA> LEU B 83 <NA> -5.463 16.644 8.357  
## 2273 ATOM 2274 CG <NA> LEU B 83 <NA> -4.590 15.919 7.327  
## 2274 ATOM 2275 CD1 <NA> LEU B 83 <NA> -5.338 14.900 6.502  
## 2275 ATOM 2276 CD2 <NA> LEU B 83 <NA> -3.961 16.966 6.435  
## 2276 ATOM 2277 N <NA> ASP B 84 <NA> -6.016 13.885 10.463  
## 2277 ATOM 2278 CA <NA> ASP B 84 <NA> -5.505 12.951 11.428  
## 2278 ATOM 2279 C <NA> ASP B 84 <NA> -4.211 12.283 10.984  
## 2279 ATOM 2280 O <NA> ASP B 84 <NA> -4.229 11.499 10.038  
## 2280 ATOM 2281 CB <NA> ASP B 84 <NA> -6.616 11.904 11.639  
## 2281 ATOM 2282 CG <NA> ASP B 84 <NA> -6.240 10.807 12.601  
## 2282 ATOM 2283 OD1 <NA> ASP B 84 <NA> -6.040 11.105 13.795  
## 2283 ATOM 2284 OD2 <NA> ASP B 84 <NA> -6.178 9.636 12.156  
## 2284 ATOM 2285 N <NA> GLY B 85 <NA> -3.088 12.612 11.629  
## 2285 ATOM 2286 CA <NA> GLY B 85 <NA> -1.824 11.955 11.308  
## 2286 ATOM 2287 C <NA> GLY B 85 <NA> -1.203 12.073 9.924  
## 2287 ATOM 2288 O <NA> GLY B 85 <NA> -0.704 11.082 9.351  
## 2288 ATOM 2289 N <NA> PHE B 86 <NA> -1.296 13.274 9.360  
## 2289 ATOM 2290 CA <NA> PHE B 86 <NA> -0.712 13.595 8.068  
## 2290 ATOM 2291 C <NA> PHE B 86 <NA> -0.545 15.086 8.165  
## 2291 ATOM 2292 O <NA> PHE B 86 <NA> -1.447 15.767 8.638  
## 2292 ATOM 2293 CB <NA> PHE B 86 <NA> -1.607 13.236 6.870  
## 2293 ATOM 2294 CG <NA> PHE B 86 <NA> -0.871 13.302 5.543  
## 2294 ATOM 2295 CD1 <NA> PHE B 86 <NA> -0.015 12.277 5.154  
## 2295 ATOM 2296 CD2 <NA> PHE B 86 <NA> -0.912 14.448 4.755  
## 2296 ATOM 2297 CE1 <NA> PHE B 86 <NA> 0.792 12.404 4.013  
## 2297 ATOM 2298 CE2 <NA> PHE B 86 <NA> -0.106 14.573 3.616  
## 2298 ATOM 2299 CZ <NA> PHE B 86 <NA> 0.741 13.556 3.252  
## 2299 ATOM 2300 N <NA> PRO B 87 <NA> 0.629 15.614 7.773  
## 2300 ATOM 2301 CA <NA> PRO B 87 <NA> 1.774 14.876 7.254  
## 2301 ATOM 2302 C <NA> PRO B 87 <NA> 2.556 14.053 8.251  
## 2302 ATOM 2303 O <NA> PRO B 87 <NA> 2.375 14.194 9.456  
## 2303 ATOM 2304 CB <NA> PRO B 87 <NA> 2.637 15.987 6.651  
## 2304 ATOM 2305 CG <NA> PRO B 87 <NA> 2.361 17.100 7.481  
## 2305 ATOM 2306 CD <NA> PRO B 87 <NA> 0.860 17.048 7.587  
## 2306 ATOM 2307 N <NA> ARG B 88 <NA> 3.381 13.158 7.711  
## 2307 ATOM 2308 CA <NA> ARG B 88 <NA> 4.272 12.295 8.475  
## 2308 ATOM 2309 C <NA> ARG B 88 <NA> 5.737 12.726 8.319  
## 2309 ATOM 2310 O <NA> ARG B 88 <NA> 6.591 12.242 9.048  
## 2310 ATOM 2311 CB <NA> ARG B 88 <NA> 4.156 10.847 8.009  
## 2311 ATOM 2312 CG <NA> ARG B 88 <NA> 2.787 10.234 8.200  
## 2312 ATOM 2313 CD <NA> ARG B 88 <NA> 2.657 8.971 7.414  
## 2313 ATOM 2314 NE <NA> ARG B 88 <NA> 1.350 8.916 6.763  
## 2314 ATOM 2315 CZ <NA> ARG B 88 <NA> 1.168 8.569 5.490  
## 2315 ATOM 2316 NH1 <NA> ARG B 88 <NA> 2.208 8.219 4.736  
## 2316 ATOM 2317 NH2 <NA> ARG B 88 <NA> -0.051 8.551 4.968  
## 2317 ATOM 2318 N <NA> THR B 89 <NA> 6.051 13.598 7.361  
## 2318 ATOM 2319 CA <NA> THR B 89 <NA> 7.443 14.034 7.178  
## 2319 ATOM 2320 C <NA> THR B 89 <NA> 7.511 15.477 6.703  
## 2320 ATOM 2321 O <NA> THR B 89 <NA> 6.510 16.025 6.280  
## 2321 ATOM 2322 CB <NA> THR B 89 <NA> 8.168 13.184 6.124  
## 2322 ATOM 2323 OG1 <NA> THR B 89 <NA> 7.441 13.240 4.893  
## 2323 ATOM 2324 CG2 <NA> THR B 89 <NA> 8.310 11.745 6.563  
## 2324 ATOM 2325 N <NA> ILE B 90 <NA> 8.695 16.078 6.717  
## 2325 ATOM 2326 CA <NA> ILE B 90 <NA> 8.843 17.463 6.254  
## 2326 ATOM 2327 C <NA> ILE B 90 <NA> 8.530 17.649 4.754  
## 2327 ATOM 2328 O <NA> ILE B 90 <NA> 7.911 18.634 4.365  
## 2328 ATOM 2329 CB <NA> ILE B 90 <NA> 10.243 18.046 6.597  
## 2329 ATOM 2330 CG1 <NA> ILE B 90 <NA> 10.408 18.161 8.111  
## 2330 ATOM 2331 CG2 <NA> ILE B 90 <NA> 10.403 19.443 6.011  
## 2331 ATOM 2332 CD1 <NA> ILE B 90 <NA> 11.815 18.556 8.545  
## 2332 ATOM 2333 N <NA> PRO B 91 <NA> 8.982 16.729 3.885  
## 2333 ATOM 2334 CA <NA> PRO B 91 <NA> 8.656 16.944 2.479  
## 2334 ATOM 2335 C <NA> PRO B 91 <NA> 7.151 16.930 2.252  
## 2335 ATOM 2336 O <NA> PRO B 91 <NA> 6.651 17.569 1.347  
## 2336 ATOM 2337 CB <NA> PRO B 91 <NA> 9.348 15.770 1.798  
## 2337 ATOM 2338 CG <NA> PRO B 91 <NA> 10.529 15.549 2.651  
## 2338 ATOM 2339 CD <NA> PRO B 91 <NA> 9.934 15.613 4.016  
## 2339 ATOM 2340 N <NA> GLN B 92 <NA> 6.423 16.187 3.067  
## 2340 ATOM 2341 CA <NA> GLN B 92 <NA> 4.974 16.135 2.935  
## 2341 ATOM 2342 C <NA> GLN B 92 <NA> 4.339 17.435 3.416  
## 2342 ATOM 2343 O <NA> GLN B 92 <NA> 3.377 17.924 2.827  
## 2343 ATOM 2344 CB <NA> GLN B 92 <NA> 4.430 14.993 3.754  
## 2344 ATOM 2345 CG <NA> GLN B 92 <NA> 4.592 13.686 3.086  
## 2345 ATOM 2346 CD <NA> GLN B 92 <NA> 4.231 12.574 3.991  
## 2346 ATOM 2347 OE1 <NA> GLN B 92 <NA> 3.975 12.786 5.155  
## 2347 ATOM 2348 NE2 <NA> GLN B 92 <NA> 4.191 11.383 3.470  
## 2348 ATOM 2349 N <NA> ALA B 93 <NA> 4.902 18.008 4.475  
## 2349 ATOM 2350 CA <NA> ALA B 93 <NA> 4.401 19.240 5.042  
## 2350 ATOM 2351 C <NA> ALA B 93 <NA> 4.682 20.410 4.087  
## 2351 ATOM 2352 O <NA> ALA B 93 <NA> 3.830 21.264 3.843  
## 2352 ATOM 2353 CB <NA> ALA B 93 <NA> 5.037 19.439 6.405  
## 2353 ATOM 2354 N <NA> ASP B 94 <NA> 5.870 20.386 3.506  
## 2354 ATOM 2355 CA <NA> ASP B 94 <NA> 6.328 21.359 2.535  
## 2355 ATOM 2356 C <NA> ASP B 94 <NA> 5.440 21.281 1.303  
## 2356 ATOM 2357 O <NA> ASP B 94 <NA> 4.999 22.298 0.795  
## 2357 ATOM 2358 CB <NA> ASP B 94 <NA> 7.750 21.007 2.111  
## 2358 ATOM 2359 CG <NA> ASP B 94 <NA> 8.691 22.167 2.198  
## 2359 ATOM 2360 OD1 <NA> ASP B 94 <NA> 8.258 23.321 1.959  
## 2360 ATOM 2361 OD2 <NA> ASP B 94 <NA> 9.876 21.912 2.507  
## 2361 ATOM 2362 N <NA> ALA B 95 <NA> 5.234 20.070 0.799  
## 2362 ATOM 2363 CA <NA> ALA B 95 <NA> 4.383 19.821 -0.359  
## 2363 ATOM 2364 C <NA> ALA B 95 <NA> 2.967 20.321 -0.081  
## 2364 ATOM 2365 O <NA> ALA B 95 <NA> 2.260 20.736 -0.998  
## 2365 ATOM 2366 CB <NA> ALA B 95 <NA> 4.344 18.345 -0.684  
## 2366 ATOM 2367 N <NA> MET B 96 <NA> 2.526 20.259 1.172  
## 2367 ATOM 2368 CA <NA> MET B 96 <NA> 1.198 20.752 1.492  
## 2368 ATOM 2369 C <NA> MET B 96 <NA> 1.175 22.259 1.365  
## 2369 ATOM 2370 O <NA> MET B 96 <NA> 0.277 22.809 0.733  
## 2370 ATOM 2371 CB <NA> MET B 96 <NA> 0.800 20.363 2.900  
## 2371 ATOM 2372 CG <NA> MET B 96 <NA> -0.120 19.164 2.935  
## 2372 ATOM 2373 SD <NA> MET B 96 <NA> -0.372 18.665 4.615  
## 2373 ATOM 2374 CE <NA> MET B 96 <NA> -1.449 19.915 5.197  
## 2374 ATOM 2375 N <NA> LYS B 97 <NA> 2.179 22.925 1.931  
## 2375 ATOM 2376 CA <NA> LYS B 97 <NA> 2.248 24.376 1.881  
## 2376 ATOM 2377 C <NA> LYS B 97 <NA> 2.336 24.929 0.452  
## 2377 ATOM 2378 O <NA> LYS B 97 <NA> 1.708 25.939 0.126  
## 2378 ATOM 2379 CB <NA> LYS B 97 <NA> 3.413 24.886 2.725  
## 2379 ATOM 2380 CG <NA> LYS B 97 <NA> 3.700 26.382 2.493  
## 2380 ATOM 2381 CD <NA> LYS B 97 <NA> 4.597 27.025 3.544  
## 2381 ATOM 2382 CE <NA> LYS B 97 <NA> 6.031 26.596 3.387  
## 2382 ATOM 2383 NZ <NA> LYS B 97 <NA> 6.879 27.333 4.367  
## 2383 ATOM 2384 N <NA> GLU B 98 <NA> 3.116 24.266 -0.397  
## 2384 ATOM 2385 CA <NA> GLU B 98 <NA> 3.275 24.680 -1.787  
## 2385 ATOM 2386 C <NA> GLU B 98 <NA> 1.986 24.571 -2.570  
## 2386 ATOM 2387 O <NA> GLU B 98 <NA> 1.664 25.471 -3.329  
## 2387 ATOM 2388 CB <NA> GLU B 98 <NA> 4.443 23.953 -2.444  
## 2388 ATOM 2389 CG <NA> GLU B 98 <NA> 5.760 24.732 -2.237  
## 2389 ATOM 2390 CD <NA> GLU B 98 <NA> 7.002 23.868 -2.297  
## 2390 ATOM 2391 OE1 <NA> GLU B 98 <NA> 6.947 22.782 -2.900  
## 2391 ATOM 2392 OE2 <NA> GLU B 98 <NA> 8.039 24.277 -1.729  
## 2392 ATOM 2393 N <NA> ALA B 99 <NA> 1.216 23.513 -2.350  
## 2393 ATOM 2394 CA <NA> ALA B 99 <NA> -0.098 23.384 -2.994  
## 2394 ATOM 2395 C <NA> ALA B 99 <NA> -1.139 24.317 -2.338  
## 2395 ATOM 2396 O <NA> ALA B 99 <NA> -2.339 24.196 -2.581  
## 2396 ATOM 2397 CB <NA> ALA B 99 <NA> -0.588 21.942 -2.940  
## 2397 ATOM 2398 N <NA> GLY B 100 <NA> -0.679 25.211 -1.469  
## 2398 ATOM 2399 CA <NA> GLY B 100 <NA> -1.567 26.142 -0.810  
## 2399 ATOM 2400 C <NA> GLY B 100 <NA> -2.468 25.596 0.275  
## 2400 ATOM 2401 O <NA> GLY B 100 <NA> -3.400 26.292 0.653  
## 2401 ATOM 2402 N <NA> ILE B 101 <NA> -2.251 24.367 0.748  
## 2402 ATOM 2403 CA <NA> ILE B 101 <NA> -3.076 23.790 1.834  
## 2403 ATOM 2404 C <NA> ILE B 101 <NA> -2.530 24.249 3.180  
## 2404 ATOM 2405 O <NA> ILE B 101 <NA> -1.494 23.763 3.642  
## 2405 ATOM 2406 CB <NA> ILE B 101 <NA> -3.047 22.241 1.869  
## 2406 ATOM 2407 CG1 <NA> ILE B 101 <NA> -3.434 21.641 0.516  
## 2407 ATOM 2408 CG2 <NA> ILE B 101 <NA> -4.029 21.736 2.921  
## 2408 ATOM 2409 CD1 <NA> ILE B 101 <NA> -2.944 20.219 0.340  
## 2409 ATOM 2410 N <NA> ASN B 102 <NA> -3.228 25.166 3.828  
## 2410 ATOM 2411 CA <NA> ASN B 102 <NA> -2.779 25.683 5.106  
## 2411 ATOM 2412 C <NA> ASN B 102 <NA> -3.639 25.213 6.252  
## 2412 ATOM 2413 O <NA> ASN B 102 <NA> -4.791 24.875 6.058  
## 2413 ATOM 2414 CB <NA> ASN B 102 <NA> -2.748 27.214 5.085  
## 2414 ATOM 2415 CG <NA> ASN B 102 <NA> -1.599 27.777 4.244  
## 2415 ATOM 2416 OD1 <NA> ASN B 102 <NA> -1.801 28.709 3.462  
## 2416 ATOM 2417 ND2 <NA> ASN B 102 <NA> -0.389 27.219 4.408  
## 2417 ATOM 2418 N <NA> VAL B 103 <NA> -3.055 25.186 7.441  
## 2418 ATOM 2419 CA <NA> VAL B 103 <NA> -3.754 24.774 8.644  
## 2419 ATOM 2420 C <NA> VAL B 103 <NA> -3.561 25.854 9.681  
## 2420 ATOM 2421 O <NA> VAL B 103 <NA> -2.577 26.580 9.676  
## 2421 ATOM 2422 CB <NA> VAL B 103 <NA> -3.238 23.448 9.195  
## 2422 ATOM 2423 CG1 <NA> VAL B 103 <NA> -3.401 22.366 8.145  
## 2423 ATOM 2424 CG2 <NA> VAL B 103 <NA> -1.780 23.592 9.614  
## 2424 ATOM 2425 N <NA> ASP B 104 <NA> -4.533 25.959 10.562  
## 2425 ATOM 2426 CA <NA> ASP B 104 <NA> -4.533 26.954 11.607  
## 2426 ATOM 2427 C <NA> ASP B 104 <NA> -3.818 26.471 12.844  
## 2427 ATOM 2428 O <NA> ASP B 104 <NA> -3.246 27.266 13.585  
## 2428 ATOM 2429 CB <NA> ASP B 104 <NA> -5.984 27.289 11.977  
## 2429 ATOM 2430 CG <NA> ASP B 104 <NA> -6.798 27.719 10.778  
## 2430 ATOM 2431 OD1 <NA> ASP B 104 <NA> -6.460 28.771 10.203  
## 2431 ATOM 2432 OD2 <NA> ASP B 104 <NA> -7.747 26.997 10.393  
## 2432 ATOM 2433 N <NA> TYR B 105 <NA> -3.903 25.176 13.104  
## 2433 ATOM 2434 CA <NA> TYR B 105 <NA> -3.305 24.624 14.295  
## 2434 ATOM 2435 C <NA> TYR B 105 <NA> -2.706 23.264 14.036  
## 2435 ATOM 2436 O <NA> TYR B 105 <NA> -3.231 22.471 13.262  
## 2436 ATOM 2437 CB <NA> TYR B 105 <NA> -4.361 24.428 15.383  
## 2437 ATOM 2438 CG <NA> TYR B 105 <NA> -4.929 25.689 15.950  
## 2438 ATOM 2439 CD1 <NA> TYR B 105 <NA> -6.006 26.329 15.327  
## 2439 ATOM 2440 CD2 <NA> TYR B 105 <NA> -4.397 26.259 17.097  
## 2440 ATOM 2441 CE1 <NA> TYR B 105 <NA> -6.535 27.519 15.830  
## 2441 ATOM 2442 CE2 <NA> TYR B 105 <NA> -4.921 27.449 17.613  
## 2442 ATOM 2443 CZ <NA> TYR B 105 <NA> -5.989 28.075 16.971  
## 2443 ATOM 2444 OH <NA> TYR B 105 <NA> -6.501 29.271 17.446  
## 2444 ATOM 2445 N <NA> VAL B 106 <NA> -1.599 23.001 14.703  
## 2445 ATOM 2446 CA <NA> VAL B 106 <NA> -0.955 21.720 14.623  
## 2446 ATOM 2447 C <NA> VAL B 106 <NA> -0.931 21.322 16.079  
## 2447 ATOM 2448 O <NA> VAL B 106 <NA> -0.348 22.015 16.908  
## 2448 ATOM 2449 CB <NA> VAL B 106 <NA> 0.439 21.833 14.083  
## 2449 ATOM 2450 CG1 <NA> VAL B 106 <NA> 1.051 20.458 14.054  
## 2450 ATOM 2451 CG2 <NA> VAL B 106 <NA> 0.388 22.416 12.686  
## 2451 ATOM 2452 N <NA> LEU B 107 <NA> -1.668 20.277 16.411  
## 2452 ATOM 2453 CA <NA> LEU B 107 <NA> -1.756 19.835 17.791  
## 2453 ATOM 2454 C <NA> LEU B 107 <NA> -0.985 18.561 18.012  
## 2454 ATOM 2455 O <NA> LEU B 107 <NA> -1.258 17.550 17.377  
## 2455 ATOM 2456 CB <NA> LEU B 107 <NA> -3.231 19.606 18.206  
## 2456 ATOM 2457 CG <NA> LEU B 107 <NA> -4.253 20.755 18.166  
## 2457 ATOM 2458 CD1 <NA> LEU B 107 <NA> -5.624 20.256 18.613  
## 2458 ATOM 2459 CD2 <NA> LEU B 107 <NA> -3.795 21.912 19.040  
## 2459 ATOM 2460 N <NA> GLU B 108 <NA> 0.003 18.617 18.889  
## 2460 ATOM 2461 CA <NA> GLU B 108 <NA> 0.747 17.416 19.214  
## 2461 ATOM 2462 C <NA> GLU B 108 <NA> 0.205 16.871 20.529  
## 2462 ATOM 2463 O <NA> GLU B 108 <NA> 0.300 17.519 21.563  
## 2463 ATOM 2464 CB <NA> GLU B 108 <NA> 2.241 17.671 19.341  
## 2464 ATOM 2465 CG <NA> GLU B 108 <NA> 2.949 16.372 19.640  
## 2465 ATOM 2466 CD <NA> GLU B 108 <NA> 4.404 16.531 19.860  
## 2466 ATOM 2467 OE1 <NA> GLU B 108 <NA> 4.839 17.679 20.080  
## 2467 ATOM 2468 OE2 <NA> GLU B 108 <NA> 5.109 15.497 19.812  
## 2468 ATOM 2469 N <NA> PHE B 109 <NA> -0.377 15.689 20.465  
## 2469 ATOM 2470 CA <NA> PHE B 109 <NA> -0.964 15.038 21.619  
## 2470 ATOM 2471 C <NA> PHE B 109 <NA> 0.120 14.208 22.299  
## 2471 ATOM 2472 O <NA> PHE B 109 <NA> 0.448 13.113 21.870  
## 2472 ATOM 2473 CB <NA> PHE B 109 <NA> -2.096 14.165 21.117  
## 2473 ATOM 2474 CG <NA> PHE B 109 <NA> -3.056 13.762 22.177  
## 2474 ATOM 2475 CD1 <NA> PHE B 109 <NA> -4.168 14.556 22.454  
## 2475 ATOM 2476 CD2 <NA> PHE B 109 <NA> -2.879 12.557 22.870  
## 2476 ATOM 2477 CE1 <NA> PHE B 109 <NA> -5.088 14.158 23.388  
## 2477 ATOM 2478 CE2 <NA> PHE B 109 <NA> -3.802 12.137 23.820  
## 2478 ATOM 2479 CZ <NA> PHE B 109 <NA> -4.913 12.937 24.081  
## 2479 ATOM 2480 N <NA> ASP B 110 <NA> 0.604 14.683 23.424  
## 2480 ATOM 2481 CA <NA> ASP B 110 <NA> 1.717 14.033 24.095  
## 2481 ATOM 2482 C <NA> ASP B 110 <NA> 1.506 13.086 25.282  
## 2482 ATOM 2483 O <NA> ASP B 110 <NA> 1.074 13.515 26.342  
## 2483 ATOM 2484 CB <NA> ASP B 110 <NA> 2.691 15.147 24.485  
## 2484 ATOM 2485 CG <NA> ASP B 110 <NA> 4.039 14.638 24.927  
## 2485 ATOM 2486 OD1 <NA> ASP B 110 <NA> 4.559 13.680 24.313  
## 2486 ATOM 2487 OD2 <NA> ASP B 110 <NA> 4.587 15.230 25.880  
## 2487 ATOM 2488 N <NA> VAL B 111 <NA> 1.871 11.818 25.104  
## 2488 ATOM 2489 CA <NA> VAL B 111 <NA> 1.807 10.781 26.145  
## 2489 ATOM 2490 C <NA> VAL B 111 <NA> 3.193 10.104 26.105  
## 2490 ATOM 2491 O <NA> VAL B 111 <NA> 3.638 9.690 25.029  
## 2491 ATOM 2492 CB <NA> VAL B 111 <NA> 0.758 9.696 25.847  
## 2492 ATOM 2493 CG1 <NA> VAL B 111 <NA> 0.738 8.677 26.965  
## 2493 ATOM 2494 CG2 <NA> VAL B 111 <NA> -0.583 10.303 25.693  
## 2494 ATOM 2495 N <NA> PRO B 112 <NA> 3.887 9.969 27.269  
## 2495 ATOM 2496 CA <NA> PRO B 112 <NA> 5.229 9.352 27.376  
## 2496 ATOM 2497 C <NA> PRO B 112 <NA> 5.231 7.921 26.922  
## 2497 ATOM 2498 O <NA> PRO B 112 <NA> 4.267 7.202 27.147  
## 2498 ATOM 2499 CB <NA> PRO B 112 <NA> 5.547 9.443 28.876  
## 2499 ATOM 2500 CG <NA> PRO B 112 <NA> 4.718 10.612 29.348  
## 2500 ATOM 2501 CD <NA> PRO B 112 <NA> 3.411 10.382 28.600  
## 2501 ATOM 2502 N <NA> ASP B 113 <NA> 6.346 7.494 26.343  
## 2502 ATOM 2503 CA <NA> ASP B 113 <NA> 6.473 6.139 25.809  
## 2503 ATOM 2504 C <NA> ASP B 113 <NA> 6.235 5.071 26.840  
## 2504 ATOM 2505 O <NA> ASP B 113 <NA> 5.772 3.976 26.528  
## 2505 ATOM 2506 CB <NA> ASP B 113 <NA> 7.855 5.923 25.164  
## 2506 ATOM 2507 CG <NA> ASP B 113 <NA> 8.065 6.758 23.902  
## 2507 ATOM 2508 OD1 <NA> ASP B 113 <NA> 7.248 7.663 23.630  
## 2508 ATOM 2509 OD2 <NA> ASP B 113 <NA> 9.056 6.511 23.178  
## 2509 ATOM 2510 N <NA> GLU B 114 <NA> 6.571 5.384 28.078  
## 2510 ATOM 2511 CA <NA> GLU B 114 <NA> 6.388 4.432 29.148  
## 2511 ATOM 2512 C <NA> GLU B 114 <NA> 4.930 4.250 29.432  
## 2512 ATOM 2513 O <NA> GLU B 114 <NA> 4.490 3.145 29.674  
## 2513 ATOM 2514 CB <NA> GLU B 114 <NA> 7.142 4.881 30.394  
## 2514 ATOM 2515 CG <NA> GLU B 114 <NA> 8.658 4.865 30.202  
## 2515 ATOM 2516 CD <NA> GLU B 114 <NA> 9.160 3.521 29.686  
## 2516 ATOM 2517 OE1 <NA> GLU B 114 <NA> 8.753 2.484 30.264  
## 2517 ATOM 2518 OE2 <NA> GLU B 114 <NA> 9.941 3.502 28.697  
## 2518 ATOM 2519 N <NA> LEU B 115 <NA> 4.171 5.330 29.371  
## 2519 ATOM 2520 CA <NA> LEU B 115 <NA> 2.745 5.250 29.622  
## 2520 ATOM 2521 C <NA> LEU B 115 <NA> 2.021 4.570 28.473  
## 2521 ATOM 2522 O <NA> LEU B 115 <NA> 1.024 3.868 28.698  
## 2522 ATOM 2523 CB <NA> LEU B 115 <NA> 2.163 6.633 29.871  
## 2523 ATOM 2524 CG <NA> LEU B 115 <NA> 2.261 7.142 31.307  
## 2524 ATOM 2525 CD1 <NA> LEU B 115 <NA> 3.678 7.059 31.814  
## 2525 ATOM 2526 CD2 <NA> LEU B 115 <NA> 1.765 8.564 31.381  
## 2526 ATOM 2527 N <NA> ILE B 116 <NA> 2.508 4.766 27.241  
## 2527 ATOM 2528 CA <NA> ILE B 116 <NA> 1.869 4.124 26.089  
## 2528 ATOM 2529 C <NA> ILE B 116 <NA> 2.178 2.646 26.191  
## 2529 ATOM 2530 O <NA> ILE B 116 <NA> 1.280 1.822 26.053  
## 2530 ATOM 2531 CB <NA> ILE B 116 <NA> 2.321 4.685 24.712  
## 2531 ATOM 2532 CG1 <NA> ILE B 116 <NA> 1.782 6.102 24.511  
## 2532 ATOM 2533 CG2 <NA> ILE B 116 <NA> 1.773 3.793 23.605  
## 2533 ATOM 2534 CD1 <NA> ILE B 116 <NA> 2.598 6.929 23.548  
## 2534 ATOM 2535 N <NA> VAL B 117 <NA> 3.440 2.308 26.460  
## 2535 ATOM 2536 CA <NA> VAL B 117 <NA> 3.823 0.908 26.641  
## 2536 ATOM 2537 C <NA> VAL B 117 <NA> 2.875 0.239 27.663  
## 2537 ATOM 2538 O <NA> VAL B 117 <NA> 2.273 -0.782 27.366  
## 2538 ATOM 2539 CB <NA> VAL B 117 <NA> 5.280 0.781 27.130  
## 2539 ATOM 2540 CG1 <NA> VAL B 117 <NA> 5.585 -0.643 27.470  
## 2540 ATOM 2541 CG2 <NA> VAL B 117 <NA> 6.233 1.248 26.056  
## 2541 ATOM 2542 N <NA> ASP B 118 <NA> 2.691 0.866 28.826  
## 2542 ATOM 2543 CA <NA> ASP B 118 <NA> 1.819 0.362 29.899  
## 2543 ATOM 2544 C <NA> ASP B 118 <NA> 0.394 0.133 29.439  
## 2544 ATOM 2545 O <NA> ASP B 118 <NA> -0.205 -0.905 29.729  
## 2545 ATOM 2546 CB <NA> ASP B 118 <NA> 1.747 1.357 31.068  
## 2546 ATOM 2547 CG <NA> ASP B 118 <NA> 3.062 1.509 31.823  
## 2547 ATOM 2548 OD1 <NA> ASP B 118 <NA> 4.052 0.777 31.531  
## 2548 ATOM 2549 OD2 <NA> ASP B 118 <NA> 3.088 2.381 32.727  
## 2549 ATOM 2550 N <NA> ARG B 119 <NA> -0.174 1.149 28.797  
## 2550 ATOM 2551 CA <NA> ARG B 119 <NA> -1.544 1.092 28.303  
## 2551 ATOM 2552 C <NA> ARG B 119 <NA> -1.740 -0.041 27.318  
## 2552 ATOM 2553 O <NA> ARG B 119 <NA> -2.843 -0.556 27.189  
## 2553 ATOM 2554 CB <NA> ARG B 119 <NA> -1.940 2.432 27.666  
## 2554 ATOM 2555 CG <NA> ARG B 119 <NA> -1.949 3.556 28.671  
## 2555 ATOM 2556 CD <NA> ARG B 119 <NA> -2.185 4.935 28.069  
## 2556 ATOM 2557 NE <NA> ARG B 119 <NA> -2.266 5.955 29.128  
## 2557 ATOM 2558 CZ <NA> ARG B 119 <NA> -2.327 7.268 28.913  
## 2558 ATOM 2559 NH1 <NA> ARG B 119 <NA> -2.303 7.738 27.672  
## 2559 ATOM 2560 NH2 <NA> ARG B 119 <NA> -2.409 8.114 29.936  
## 2560 ATOM 2561 N <NA> ILE B 120 <NA> -0.655 -0.480 26.686  
## 2561 ATOM 2562 CA <NA> ILE B 120 <NA> -0.723 -1.537 25.693  
## 2562 ATOM 2563 C <NA> ILE B 120 <NA> -0.286 -2.946 26.117  
## 2563 ATOM 2564 O <NA> ILE B 120 <NA> -0.984 -3.914 25.810  
## 2564 ATOM 2565 CB <NA> ILE B 120 <NA> 0.014 -1.110 24.426  
## 2565 ATOM 2566 CG1 <NA> ILE B 120 <NA> -0.637 0.151 23.853  
## 2566 ATOM 2567 CG2 <NA> ILE B 120 <NA> -0.002 -2.227 23.408  
## 2567 ATOM 2568 CD1 <NA> ILE B 120 <NA> 0.037 0.685 22.610  
## 2568 ATOM 2569 N <NA> VAL B 121 <NA> 0.851 -3.093 26.800  
## 2569 ATOM 2570 CA <NA> VAL B 121 <NA> 1.289 -4.437 27.216  
## 2570 ATOM 2571 C <NA> VAL B 121 <NA> 0.353 -5.105 28.244  
## 2571 ATOM 2572 O <NA> VAL B 121 <NA> 0.187 -6.339 28.240  
## 2572 ATOM 2573 CB <NA> VAL B 121 <NA> 2.762 -4.479 27.726  
## 2573 ATOM 2574 CG1 <NA> VAL B 121 <NA> 3.682 -3.811 26.711  
## 2574 ATOM 2575 CG2 <NA> VAL B 121 <NA> 2.884 -3.883 29.129  
## 2575 ATOM 2576 N <NA> GLY B 122 <NA> -0.253 -4.295 29.115  
## 2576 ATOM 2577 CA <NA> GLY B 122 <NA> -1.175 -4.826 30.102  
## 2577 ATOM 2578 C <NA> GLY B 122 <NA> -2.566 -4.903 29.497  
## 2578 ATOM 2579 O <NA> GLY B 122 <NA> -3.533 -4.442 30.091  
## 2579 ATOM 2580 N <NA> ARG B 123 <NA> -2.668 -5.511 28.323  
## 2580 ATOM 2581 CA <NA> ARG B 123 <NA> -3.929 -5.634 27.609  
## 2581 ATOM 2582 C <NA> ARG B 123 <NA> -4.206 -7.092 27.222  
## 2582 ATOM 2583 O <NA> ARG B 123 <NA> -3.387 -7.745 26.565  
## 2583 ATOM 2584 CB <NA> ARG B 123 <NA> -3.888 -4.725 26.375  
## 2584 ATOM 2585 CG <NA> ARG B 123 <NA> -4.998 -4.939 25.391  
## 2585 ATOM 2586 CD <NA> ARG B 123 <NA> -5.348 -3.655 24.674  
## 2586 ATOM 2587 NE <NA> ARG B 123 <NA> -4.411 -3.305 23.615  
## 2587 ATOM 2588 CZ <NA> ARG B 123 <NA> -4.344 -2.100 23.053  
## 2588 ATOM 2589 NH1 <NA> ARG B 123 <NA> -5.153 -1.127 23.467  
## 2589 ATOM 2590 NH2 <NA> ARG B 123 <NA> -3.458 -1.863 22.089  
## 2590 ATOM 2591 N <NA> ARG B 124 <NA> -5.349 -7.603 27.674  
## 2591 ATOM 2592 CA <NA> ARG B 124 <NA> -5.765 -8.979 27.404  
## 2592 ATOM 2593 C <NA> ARG B 124 <NA> -6.963 -8.961 26.454  
## 2593 ATOM 2594 O <NA> ARG B 124 <NA> -7.742 -7.998 26.427  
## 2594 ATOM 2595 CB <NA> ARG B 124 <NA> -6.164 -9.694 28.706  
## 2595 ATOM 2596 CG <NA> ARG B 124 <NA> -5.092 -9.761 29.782  
## 2596 ATOM 2597 CD <NA> ARG B 124 <NA> -4.065 -10.839 29.507  
## 2597 ATOM 2598 NE <NA> ARG B 124 <NA> -2.971 -10.843 30.482  
## 2598 ATOM 2599 CZ <NA> ARG B 124 <NA> -2.000 -9.928 30.544  
## 2599 ATOM 2600 NH1 <NA> ARG B 124 <NA> -1.982 -8.895 29.708  
## 2600 ATOM 2601 NH2 <NA> ARG B 124 <NA> -1.048 -10.033 31.466  
## 2601 ATOM 2602 N <NA> VAL B 125 <NA> -7.132 -10.044 25.706  
## 2602 ATOM 2603 CA <NA> VAL B 125 <NA> -8.225 -10.138 24.756  
## 2603 ATOM 2604 C <NA> VAL B 125 <NA> -8.790 -11.527 24.651  
## 2604 ATOM 2605 O <NA> VAL B 125 <NA> -8.076 -12.508 24.789  
## 2605 ATOM 2606 CB <NA> VAL B 125 <NA> -7.805 -9.724 23.330  
## 2606 ATOM 2607 CG1 <NA> VAL B 125 <NA> -7.956 -8.230 23.146  
## 2607 ATOM 2608 CG2 <NA> VAL B 125 <NA> -6.372 -10.178 23.044  
## 2608 ATOM 2609 N <NA> HIS B 126 <NA> -10.097 -11.595 24.429  
## 2609 ATOM 2610 CA <NA> HIS B 126 <NA> -10.768 -12.864 24.250  
## 2610 ATOM 2611 C <NA> HIS B 126 <NA> -10.626 -13.139 22.770  
## 2611 ATOM 2612 O <NA> HIS B 126 <NA> -11.407 -12.635 21.957  
## 2612 ATOM 2613 CB <NA> HIS B 126 <NA> -12.249 -12.789 24.601  
## 2613 ATOM 2614 CG <NA> HIS B 126 <NA> -12.970 -14.064 24.314  
## 2614 ATOM 2615 ND1 <NA> HIS B 126 <NA> -12.757 -15.214 25.043  
## 2615 ATOM 2616 CD2 <NA> HIS B 126 <NA> -13.817 -14.405 23.314  
## 2616 ATOM 2617 CE1 <NA> HIS B 126 <NA> -13.435 -16.208 24.501  
## 2617 ATOM 2618 NE2 <NA> HIS B 126 <NA> -14.090 -15.743 23.452  
## 2618 ATOM 2619 N <NA> ALA B 127 <NA> -9.640 -13.961 22.440  
## 2619 ATOM 2620 CA <NA> ALA B 127 <NA> -9.332 -14.299 21.060  
## 2620 ATOM 2621 C <NA> ALA B 127 <NA> -10.516 -14.492 20.099  
## 2621 ATOM 2622 O <NA> ALA B 127 <NA> -10.623 -13.772 19.100  
## 2622 ATOM 2623 CB <NA> ALA B 127 <NA> -8.380 -15.494 21.015  
## 2623 ATOM 2624 N <NA> PRO B 128 <NA> -11.453 -15.410 20.418  
## 2624 ATOM 2625 CA <NA> PRO B 128 <NA> -12.612 -15.658 19.545  
## 2625 ATOM 2626 C <NA> PRO B 128 <NA> -13.568 -14.493 19.223  
## 2626 ATOM 2627 O <NA> PRO B 128 <NA> -14.286 -14.544 18.222  
## 2627 ATOM 2628 CB <NA> PRO B 128 <NA> -13.338 -16.800 20.267  
## 2628 ATOM 2629 CG <NA> PRO B 128 <NA> -12.220 -17.538 20.940  
## 2629 ATOM 2630 CD <NA> PRO B 128 <NA> -11.420 -16.396 21.516  
## 2630 ATOM 2631 N <NA> SER B 129 <NA> -13.580 -13.449 20.046  
## 2631 ATOM 2632 CA <NA> SER B 129 <NA> -14.481 -12.318 19.815  
## 2632 ATOM 2633 C <NA> SER B 129 <NA> -13.752 -10.988 19.705  
## 2633 ATOM 2634 O <NA> SER B 129 <NA> -14.355 -9.965 19.348  
## 2634 ATOM 2635 CB <NA> SER B 129 <NA> -15.476 -12.222 20.963  
## 2635 ATOM 2636 OG <NA> SER B 129 <NA> -14.784 -12.090 22.196  
## 2636 ATOM 2637 N <NA> GLY B 130 <NA> -12.472 -11.006 20.066  
## 2637 ATOM 2638 CA <NA> GLY B 130 <NA> -11.669 -9.803 20.036  
## 2638 ATOM 2639 C <NA> GLY B 130 <NA> -12.024 -8.860 21.175  
## 2639 ATOM 2640 O <NA> GLY B 130 <NA> -11.605 -7.699 21.160  
## 2640 ATOM 2641 N <NA> ARG B 131 <NA> -12.786 -9.343 22.162  
## 2641 ATOM 2642 CA <NA> ARG B 131 <NA> -13.185 -8.518 23.311  
## 2642 ATOM 2643 C <NA> ARG B 131 <NA> -11.974 -8.143 24.166  
## 2643 ATOM 2644 O <NA> ARG B 131 <NA> -11.232 -9.005 24.639  
## 2644 ATOM 2645 CB <NA> ARG B 131 <NA> -14.262 -9.213 24.155  
## 2645 ATOM 2646 CG <NA> ARG B 131 <NA> -15.670 -9.136 23.555  
## 2646 ATOM 2647 CD <NA> ARG B 131 <NA> -16.721 -9.788 24.456  
## 2647 ATOM 2648 NE <NA> ARG B 131 <NA> -16.543 -11.237 24.598  
## 2648 ATOM 2649 CZ <NA> ARG B 131 <NA> -17.201 -12.153 23.887  
## 2649 ATOM 2650 NH1 <NA> ARG B 131 <NA> -18.062 -11.783 22.948  
## 2650 ATOM 2651 NH2 <NA> ARG B 131 <NA> -16.974 -13.444 24.090  
## 2651 ATOM 2652 N <NA> VAL B 132 <NA> -11.796 -6.846 24.366  
## 2652 ATOM 2653 CA <NA> VAL B 132 <NA> -10.664 -6.319 25.103  
## 2653 ATOM 2654 C <NA> VAL B 132 <NA> -10.863 -6.139 26.606  
## 2654 ATOM 2655 O <NA> VAL B 132 <NA> -11.958 -5.800 27.068  
## 2655 ATOM 2656 CB <NA> VAL B 132 <NA> -10.211 -4.976 24.464  
## 2656 ATOM 2657 CG1 <NA> VAL B 132 <NA> -9.101 -4.325 25.282  
## 2657 ATOM 2658 CG2 <NA> VAL B 132 <NA> -9.744 -5.206 23.023  
## 2658 ATOM 2659 N <NA> TYR B 133 <NA> -9.774 -6.346 27.344  
## 2659 ATOM 2660 CA <NA> TYR B 133 <NA> -9.712 -6.204 28.795  
## 2660 ATOM 2661 C <NA> TYR B 133 <NA> -8.345 -5.589 29.105  
## 2661 ATOM 2662 O <NA> TYR B 133 <NA> -7.392 -5.788 28.352  
## 2662 ATOM 2663 CB <NA> TYR B 133 <NA> -9.788 -7.581 29.484  
## 2663 ATOM 2664 CG <NA> TYR B 133 <NA> -11.111 -8.279 29.341  
## 2664 ATOM 2665 CD1 <NA> TYR B 133 <NA> -12.260 -7.725 29.893  
## 2665 ATOM 2666 CD2 <NA> TYR B 133 <NA> -11.234 -9.439 28.588  
## 2666 ATOM 2667 CE1 <NA> TYR B 133 <NA> -13.511 -8.296 29.690  
## 2667 ATOM 2668 CE2 <NA> TYR B 133 <NA> -12.483 -10.028 28.374  
## 2668 ATOM 2669 CZ <NA> TYR B 133 <NA> -13.626 -9.445 28.925  
## 2669 ATOM 2670 OH <NA> TYR B 133 <NA> -14.893 -9.954 28.678  
## 2670 ATOM 2671 N <NA> HIS B 134 <NA> -8.253 -4.822 30.187  
## 2671 ATOM 2672 CA <NA> HIS B 134 <NA> -6.982 -4.239 30.595  
## 2672 ATOM 2673 C <NA> HIS B 134 <NA> -6.734 -4.382 32.097  
## 2673 ATOM 2674 O <NA> HIS B 134 <NA> -7.240 -3.596 32.906  
## 2674 ATOM 2675 CB <NA> HIS B 134 <NA> -6.834 -2.772 30.184  
## 2675 ATOM 2676 CG <NA> HIS B 134 <NA> -5.433 -2.271 30.337  
## 2676 ATOM 2677 ND1 <NA> HIS B 134 <NA> -4.798 -2.210 31.560  
## 2677 ATOM 2678 CD2 <NA> HIS B 134 <NA> -4.495 -1.946 29.416  
## 2678 ATOM 2679 CE1 <NA> HIS B 134 <NA> -3.531 -1.884 31.384  
## 2679 ATOM 2680 NE2 <NA> HIS B 134 <NA> -3.321 -1.718 30.093  
## 2680 ATOM 2681 N <NA> VAL B 135 <NA> -5.824 -5.296 32.424  
## 2681 ATOM 2682 CA <NA> VAL B 135 <NA> -5.435 -5.638 33.800  
## 2682 ATOM 2683 C <NA> VAL B 135 <NA> -5.466 -4.554 34.886  
## 2683 ATOM 2684 O <NA> VAL B 135 <NA> -5.882 -4.810 36.014  
## 2684 ATOM 2685 CB <NA> VAL B 135 <NA> -4.058 -6.384 33.838  
## 2685 ATOM 2686 CG1 <NA> VAL B 135 <NA> -4.161 -7.696 33.091  
## 2686 ATOM 2687 CG2 <NA> VAL B 135 <NA> -2.954 -5.537 33.246  
## 2687 ATOM 2688 N <NA> LYS B 136 <NA> -5.010 -3.355 34.559  
## 2688 ATOM 2689 CA <NA> LYS B 136 <NA> -5.013 -2.290 35.544  
## 2689 ATOM 2690 C <NA> LYS B 136 <NA> -6.251 -1.418 35.406  
## 2690 ATOM 2691 O <NA> LYS B 136 <NA> -6.789 -0.927 36.397  
## 2691 ATOM 2692 CB <NA> LYS B 136 <NA> -3.747 -1.433 35.412  
## 2692 ATOM 2693 CG <NA> LYS B 136 <NA> -2.427 -2.192 35.578  
## 2693 ATOM 2694 CD <NA> LYS B 136 <NA> -1.840 -2.613 34.237  
## 2694 ATOM 2695 CE <NA> LYS B 136 <NA> -0.521 -3.364 34.399  
## 2695 ATOM 2696 NZ <NA> LYS B 136 <NA> 0.111 -3.672 33.077  
## 2696 ATOM 2697 N <NA> PHE B 137 <NA> -6.680 -1.215 34.166  
## 2697 ATOM 2698 CA <NA> PHE B 137 <NA> -7.832 -0.385 33.894  
## 2698 ATOM 2699 C <NA> PHE B 137 <NA> -9.052 -1.246 34.055  
## 2699 ATOM 2700 O <NA> PHE B 137 <NA> -9.438 -1.557 35.166  
## 2700 ATOM 2701 CB <NA> PHE B 137 <NA> -7.789 0.165 32.473  
## 2701 ATOM 2702 CG <NA> PHE B 137 <NA> -6.649 1.094 32.209  
## 2702 ATOM 2703 CD1 <NA> PHE B 137 <NA> -5.414 0.913 32.834  
## 2703 ATOM 2704 CD2 <NA> PHE B 137 <NA> -6.804 2.154 31.313  
## 2704 ATOM 2705 CE1 <NA> PHE B 137 <NA> -4.351 1.767 32.577  
## 2705 ATOM 2706 CE2 <NA> PHE B 137 <NA> -5.748 3.023 31.042  
## 2706 ATOM 2707 CZ <NA> PHE B 137 <NA> -4.516 2.827 31.676  
## 2707 ATOM 2708 N <NA> ASN B 138 <NA> -9.608 -1.680 32.933  
## 2708 ATOM 2709 CA <NA> ASN B 138 <NA> -10.812 -2.503 32.883  
## 2709 ATOM 2710 C <NA> ASN B 138 <NA> -10.501 -3.999 32.961  
## 2710 ATOM 2711 O <NA> ASN B 138 <NA> -10.472 -4.699 31.939  
## 2711 ATOM 2712 CB <NA> ASN B 138 <NA> -11.575 -2.201 31.585  
## 2712 ATOM 2713 CG <NA> ASN B 138 <NA> -10.683 -2.294 30.338  
## 2713 ATOM 2714 OD1 <NA> ASN B 138 <NA> -9.687 -1.569 30.215  
## 2714 ATOM 2715 ND2 <NA> ASN B 138 <NA> -11.029 -3.194 29.419  
## 2715 ATOM 2716 N <NA> PRO B 139 <NA> -10.321 -4.525 34.172  
## 2716 ATOM 2717 CA <NA> PRO B 139 <NA> -10.017 -5.948 34.258  
## 2717 ATOM 2718 C <NA> PRO B 139 <NA> -11.247 -6.801 33.986  
## 2718 ATOM 2719 O <NA> PRO B 139 <NA> -12.383 -6.298 33.971  
## 2719 ATOM 2720 CB <NA> PRO B 139 <NA> -9.573 -6.085 35.699  
## 2720 ATOM 2721 CG <NA> PRO B 139 <NA> -10.537 -5.192 36.394  
## 2721 ATOM 2722 CD <NA> PRO B 139 <NA> -10.567 -3.967 35.512  
## 2722 ATOM 2723 N <NA> PRO B 140 <NA> -11.037 -8.087 33.669  
## 2723 ATOM 2724 CA <NA> PRO B 140 <NA> -12.222 -8.903 33.427  
## 2724 ATOM 2725 C <NA> PRO B 140 <NA> -12.771 -9.174 34.824  
## 2725 ATOM 2726 O <NA> PRO B 140 <NA> -11.993 -9.313 35.774  
## 2726 ATOM 2727 CB <NA> PRO B 140 <NA> -11.643 -10.154 32.770  
## 2727 ATOM 2728 CG <NA> PRO B 140 <NA> -10.293 -10.269 33.386  
## 2728 ATOM 2729 CD <NA> PRO B 140 <NA> -9.799 -8.850 33.429  
## 2729 ATOM 2730 N <NA> LYS B 141 <NA> -14.091 -9.139 34.983  
## 2730 ATOM 2731 CA <NA> LYS B 141 <NA> -14.688 -9.391 36.293  
## 2731 ATOM 2732 C <NA> LYS B 141 <NA> -14.061 -10.658 36.878  
## 2732 ATOM 2733 O <NA> LYS B 141 <NA> -13.668 -10.697 38.044  
## 2733 ATOM 2734 CB <NA> LYS B 141 <NA> -16.212 -9.565 36.188  
## 2734 ATOM 2735 CG <NA> LYS B 141 <NA> -17.006 -8.331 35.728  
## 2735 ATOM 2736 CD <NA> LYS B 141 <NA> -18.426 -8.346 36.330  
## 2736 ATOM 2737 CE <NA> LYS B 141 <NA> -19.371 -7.328 35.687  
## 2737 ATOM 2738 NZ <NA> LYS B 141 <NA> -19.838 -7.755 34.331  
## 2738 ATOM 2739 N <NA> VAL B 142 <NA> -13.922 -11.664 36.019  
## 2739 ATOM 2740 CA <NA> VAL B 142 <NA> -13.336 -12.952 36.378  
## 2740 ATOM 2741 C <NA> VAL B 142 <NA> -11.871 -12.904 35.922  
## 2741 ATOM 2742 O <NA> VAL B 142 <NA> -11.602 -12.915 34.717  
## 2742 ATOM 2743 CB <NA> VAL B 142 <NA> -14.060 -14.113 35.638  
## 2743 ATOM 2744 CG1 <NA> VAL B 142 <NA> -14.181 -15.329 36.554  
## 2744 ATOM 2745 CG2 <NA> VAL B 142 <NA> -15.432 -13.665 35.120  
## 2745 ATOM 2746 N <NA> GLU B 143 <NA> -10.940 -12.858 36.878  
## 2746 ATOM 2747 CA <NA> GLU B 143 <NA> -9.499 -12.765 36.590  
## 2747 ATOM 2748 C <NA> GLU B 143 <NA> -8.899 -13.766 35.585  
## 2748 ATOM 2749 O <NA> GLU B 143 <NA> -8.846 -14.973 35.829  
## 2749 ATOM 2750 CB <NA> GLU B 143 <NA> -8.684 -12.760 37.889  
## 2750 ATOM 2751 CG <NA> GLU B 143 <NA> -8.871 -13.994 38.771  
## 2751 ATOM 2752 CD <NA> GLU B 143 <NA> -7.823 -14.103 39.876  
## 2752 ATOM 2753 OE1 <NA> GLU B 143 <NA> -7.479 -13.071 40.498  
## 2753 ATOM 2754 OE2 <NA> GLU B 143 <NA> -7.343 -15.231 40.123  
## 2754 ATOM 2755 N <NA> GLY B 144 <NA> -8.409 -13.221 34.470  
## 2755 ATOM 2756 CA <NA> GLY B 144 <NA> -7.817 -14.014 33.404  
## 2756 ATOM 2757 C <NA> GLY B 144 <NA> -8.868 -14.690 32.543  
## 2757 ATOM 2758 O <NA> GLY B 144 <NA> -8.528 -15.412 31.607  
## 2758 ATOM 2759 N <NA> LYS B 145 <NA> -10.137 -14.367 32.789  
## 2759 ATOM 2760 CA <NA> LYS B 145 <NA> -11.251 -14.991 32.083  
## 2760 ATOM 2761 C <NA> LYS B 145 <NA> -12.266 -14.055 31.451  
## 2761 ATOM 2762 O <NA> LYS B 145 <NA> -12.566 -12.975 31.970  
## 2762 ATOM 2763 CB <NA> LYS B 145 <NA> -12.019 -15.901 33.040  
## 2763 ATOM 2764 CG <NA> LYS B 145 <NA> -11.159 -16.720 33.993  
## 2764 ATOM 2765 CD <NA> LYS B 145 <NA> -10.792 -18.057 33.423  
## 2765 ATOM 2766 CE <NA> LYS B 145 <NA> -10.148 -18.904 34.476  
## 2766 ATOM 2767 NZ <NA> LYS B 145 <NA> -10.035 -20.275 33.945  
## 2767 ATOM 2768 N <NA> ASP B 146 <NA> -12.843 -14.539 30.354  
## 2768 ATOM 2769 CA <NA> ASP B 146 <NA> -13.870 -13.828 29.605  
## 2769 ATOM 2770 C <NA> ASP B 146 <NA> -15.162 -13.940 30.418  
## 2770 ATOM 2771 O <NA> ASP B 146 <NA> -15.769 -15.000 30.497  
## 2771 ATOM 2772 CB <NA> ASP B 146 <NA> -14.046 -14.465 28.212  
## 2772 ATOM 2773 CG <NA> ASP B 146 <NA> -14.933 -13.640 27.281  
## 2773 ATOM 2774 OD1 <NA> ASP B 146 <NA> -14.850 -12.394 27.285  
## 2774 ATOM 2775 OD2 <NA> ASP B 146 <NA> -15.711 -14.242 26.518  
## 2775 ATOM 2776 N <NA> ASP B 147 <NA> -15.563 -12.831 31.018  
## 2776 ATOM 2777 CA <NA> ASP B 147 <NA> -16.764 -12.747 31.842  
## 2777 ATOM 2778 C <NA> ASP B 147 <NA> -17.962 -13.477 31.235  
## 2778 ATOM 2779 O <NA> ASP B 147 <NA> -18.767 -14.099 31.935  
## 2779 ATOM 2780 CB <NA> ASP B 147 <NA> -17.111 -11.274 32.039  
## 2780 ATOM 2781 CG <NA> ASP B 147 <NA> -15.921 -10.448 32.468  
## 2781 ATOM 2782 OD1 <NA> ASP B 147 <NA> -14.844 -11.022 32.729  
## 2782 ATOM 2783 OD2 <NA> ASP B 147 <NA> -16.064 -9.217 32.553  
## 2783 ATOM 2784 N <NA> VAL B 148 <NA> -18.081 -13.355 29.920  
## 2784 ATOM 2785 CA <NA> VAL B 148 <NA> -19.159 -13.987 29.176  
## 2785 ATOM 2786 C <NA> VAL B 148 <NA> -18.917 -15.480 28.954  
## 2786 ATOM 2787 O <NA> VAL B 148 <NA> -19.411 -16.308 29.714  
## 2787 ATOM 2788 CB <NA> VAL B 148 <NA> -19.483 -13.216 27.825  
## 2788 ATOM 2789 CG1 <NA> VAL B 148 <NA> -18.236 -12.559 27.260  
## 2789 ATOM 2790 CG2 <NA> VAL B 148 <NA> -20.139 -14.142 26.772  
## 2790 ATOM 2791 N <NA> THR B 149 <NA> -18.102 -15.824 27.968  
## 2791 ATOM 2792 CA <NA> THR B 149 <NA> -17.860 -17.225 27.668  
## 2792 ATOM 2793 C <NA> THR B 149 <NA> -17.197 -17.985 28.812  
## 2793 ATOM 2794 O <NA> THR B 149 <NA> -17.469 -19.165 29.042  
## 2794 ATOM 2795 CB <NA> THR B 149 <NA> -16.999 -17.374 26.394  
## 2795 ATOM 2796 OG1 <NA> THR B 149 <NA> -15.724 -16.750 26.600  
## 2796 ATOM 2797 CG2 <NA> THR B 149 <NA> -17.695 -16.730 25.195  
## 2797 ATOM 2798 N <NA> GLY B 150 <NA> -16.321 -17.292 29.525  
## 2798 ATOM 2799 CA <NA> GLY B 150 <NA> -15.587 -17.917 30.603  
## 2799 ATOM 2800 C <NA> GLY B 150 <NA> -14.194 -18.225 30.076  
## 2800 ATOM 2801 O <NA> GLY B 150 <NA> -13.224 -18.206 30.831  
## 2801 ATOM 2802 N <NA> GLU B 151 <NA> -14.097 -18.462 28.765  
## 2802 ATOM 2803 CA <NA> GLU B 151 <NA> -12.833 -18.782 28.088  
## 2803 ATOM 2804 C <NA> GLU B 151 <NA> -11.696 -17.805 28.404  
## 2804 ATOM 2805 O <NA> GLU B 151 <NA> -11.888 -16.582 28.390  
## 2805 ATOM 2806 CB <NA> GLU B 151 <NA> -13.058 -18.887 26.576  
## 2806 ATOM 2807 CG <NA> GLU B 151 <NA> -14.173 -19.864 26.207  
## 2807 ATOM 2808 CD <NA> GLU B 151 <NA> -14.352 -20.033 24.715  
## 2808 ATOM 2809 OE1 <NA> GLU B 151 <NA> -13.696 -20.931 24.149  
## 2809 ATOM 2810 OE2 <NA> GLU B 151 <NA> -15.154 -19.286 24.112  
## 2810 ATOM 2811 N <NA> GLU B 152 <NA> -10.515 -18.366 28.664  
## 2811 ATOM 2812 CA <NA> GLU B 152 <NA> -9.321 -17.603 29.021  
## 2812 ATOM 2813 C <NA> GLU B 152 <NA> -8.821 -16.610 27.985  
## 2813 ATOM 2814 O <NA> GLU B 152 <NA> -8.782 -16.894 26.778  
## 2814 ATOM 2815 CB <NA> GLU B 152 <NA> -8.182 -18.538 29.413  
## 2815 ATOM 2816 CG <NA> GLU B 152 <NA> -6.970 -17.810 29.973  
## 2816 ATOM 2817 CD <NA> GLU B 152 <NA> -5.823 -18.745 30.303  
## 2817 ATOM 2818 OE1 <NA> GLU B 152 <NA> -5.066 -19.112 29.374  
## 2818 ATOM 2819 OE2 <NA> GLU B 152 <NA> -5.679 -19.106 31.494  
## 2819 ATOM 2820 N <NA> LEU B 153 <NA> -8.396 -15.459 28.495  
## 2820 ATOM 2821 CA <NA> LEU B 153 <NA> -7.895 -14.367 27.682  
## 2821 ATOM 2822 C <NA> LEU B 153 <NA> -6.480 -14.617 27.181  
## 2822 ATOM 2823 O <NA> LEU B 153 <NA> -5.656 -15.247 27.852  
## 2823 ATOM 2824 CB <NA> LEU B 153 <NA> -7.925 -13.057 28.473  
## 2824 ATOM 2825 CG <NA> LEU B 153 <NA> -9.247 -12.720 29.154  
## 2825 ATOM 2826 CD1 <NA> LEU B 153 <NA> -9.110 -11.473 30.009  
## 2826 ATOM 2827 CD2 <NA> LEU B 153 <NA> -10.310 -12.555 28.104  
## 2827 ATOM 2828 N <NA> THR B 154 <NA> -6.226 -14.122 25.975  
## 2828 ATOM 2829 CA <NA> THR B 154 <NA> -4.932 -14.222 25.316  
## 2829 ATOM 2830 C <NA> THR B 154 <NA> -4.451 -12.794 25.090  
## 2830 ATOM 2831 O <NA> THR B 154 <NA> -5.191 -11.821 25.300  
## 2831 ATOM 2832 CB <NA> THR B 154 <NA> -5.042 -14.907 23.939  
## 2832 ATOM 2833 OG1 <NA> THR B 154 <NA> -5.920 -14.146 23.094  
## 2833 ATOM 2834 CG2 <NA> THR B 154 <NA> -5.571 -16.325 24.089  
## 2834 ATOM 2835 N <NA> THR B 155 <NA> -3.217 -12.669 24.639  
## 2835 ATOM 2836 CA <NA> THR B 155 <NA> -2.657 -11.364 24.389  
## 2836 ATOM 2837 C <NA> THR B 155 <NA> -2.389 -11.315 22.889  
## 2837 ATOM 2838 O <NA> THR B 155 <NA> -2.195 -12.361 22.258  
## 2838 ATOM 2839 CB <NA> THR B 155 <NA> -1.382 -11.169 25.235  
## 2839 ATOM 2840 OG1 <NA> THR B 155 <NA> -0.774 -9.908 24.932  
## 2840 ATOM 2841 CG2 <NA> THR B 155 <NA> -0.404 -12.304 24.993  
## 2841 ATOM 2842 N <NA> ARG B 156 <NA> -2.475 -10.123 22.305  
## 2842 ATOM 2843 CA <NA> ARG B 156 <NA> -2.228 -9.971 20.877  
## 2843 ATOM 2844 C <NA> ARG B 156 <NA> -0.740 -9.861 20.552  
## 2844 ATOM 2845 O <NA> ARG B 156 <NA> 0.022 -9.168 21.229  
## 2845 ATOM 2846 CB <NA> ARG B 156 <NA> -2.947 -8.753 20.330  
## 2846 ATOM 2847 CG <NA> ARG B 156 <NA> -3.086 -8.780 18.828  
## 2847 ATOM 2848 CD <NA> ARG B 156 <NA> -3.494 -7.426 18.258  
## 2848 ATOM 2849 NE <NA> ARG B 156 <NA> -4.110 -6.559 19.256  
## 2849 ATOM 2850 CZ <NA> ARG B 156 <NA> -5.344 -6.700 19.724  
## 2850 ATOM 2851 NH1 <NA> ARG B 156 <NA> -6.125 -7.681 19.281  
## 2851 ATOM 2852 NH2 <NA> ARG B 156 <NA> -5.794 -5.852 20.641  
## 2852 ATOM 2853 N <NA> LYS B 157 <NA> -0.340 -10.542 19.488  
## 2853 ATOM 2854 CA <NA> LYS B 157 <NA> 1.044 -10.539 19.031  
## 2854 ATOM 2855 C <NA> LYS B 157 <NA> 1.538 -9.094 18.968  
## 2855 ATOM 2856 O <NA> LYS B 157 <NA> 2.636 -8.771 19.413  
## 2856 ATOM 2857 CB <NA> LYS B 157 <NA> 1.105 -11.168 17.634  
## 2857 ATOM 2858 CG <NA> LYS B 157 <NA> 2.503 -11.440 17.102  
## 2858 ATOM 2859 CD <NA> LYS B 157 <NA> 3.170 -12.601 17.838  
## 2859 ATOM 2860 CE <NA> LYS B 157 <NA> 4.573 -12.888 17.297  
## 2860 ATOM 2861 NZ <NA> LYS B 157 <NA> 4.570 -13.311 15.863  
## 2861 ATOM 2862 N <NA> ASP B 158 <NA> 0.647 -8.224 18.511  
## 2862 ATOM 2863 CA <NA> ASP B 158 <NA> 0.916 -6.803 18.332  
## 2863 ATOM 2864 C <NA> ASP B 158 <NA> 1.176 -5.973 19.580  
## 2864 ATOM 2865 O <NA> ASP B 158 <NA> 1.882 -4.962 19.513  
## 2865 ATOM 2866 CB <NA> ASP B 158 <NA> -0.233 -6.174 17.556  
## 2866 ATOM 2867 CG <NA> ASP B 158 <NA> -0.486 -6.864 16.228  
## 2867 ATOM 2868 OD1 <NA> ASP B 158 <NA> -0.731 -8.100 16.219  
## 2868 ATOM 2869 OD2 <NA> ASP B 158 <NA> -0.444 -6.160 15.191  
## 2869 ATOM 2870 N <NA> ASP B 159 <NA> 0.599 -6.375 20.706  
## 2870 ATOM 2871 CA <NA> ASP B 159 <NA> 0.770 -5.630 21.947  
## 2871 ATOM 2872 C <NA> ASP B 159 <NA> 2.023 -6.005 22.728  
## 2872 ATOM 2873 O <NA> ASP B 159 <NA> 2.137 -5.703 23.910  
## 2873 ATOM 2874 CB <NA> ASP B 159 <NA> -0.463 -5.796 22.826  
## 2874 ATOM 2875 CG <NA> ASP B 159 <NA> -1.737 -5.408 22.115  
## 2875 ATOM 2876 OD1 <NA> ASP B 159 <NA> -1.675 -4.544 21.211  
## 2876 ATOM 2877 OD2 <NA> ASP B 159 <NA> -2.805 -5.960 22.467  
## 2877 ATOM 2878 N <NA> GLN B 160 <NA> 2.961 -6.674 22.077  
## 2878 ATOM 2879 CA <NA> GLN B 160 <NA> 4.193 -7.053 22.746  
## 2879 ATOM 2880 C <NA> GLN B 160 <NA> 5.106 -5.878 22.995  
## 2880 ATOM 2881 O <NA> GLN B 160 <NA> 5.487 -5.185 22.069  
## 2881 ATOM 2882 CB <NA> GLN B 160 <NA> 4.949 -8.083 21.932  
## 2882 ATOM 2883 CG <NA> GLN B 160 <NA> 4.302 -9.420 21.962  
## 2883 ATOM 2884 CD <NA> GLN B 160 <NA> 5.102 -10.427 21.204  
## 2884 ATOM 2885 OE1 <NA> GLN B 160 <NA> 6.131 -10.096 20.605  
## 2885 ATOM 2886 NE2 <NA> GLN B 160 <NA> 4.652 -11.680 21.232  
## 2886 ATOM 2887 N <NA> GLU B 161 <NA> 5.494 -5.703 24.248  
## 2887 ATOM 2888 CA <NA> GLU B 161 <NA> 6.388 -4.634 24.668  
## 2888 ATOM 2889 C <NA> GLU B 161 <NA> 7.527 -4.373 23.682  
## 2889 ATOM 2890 O <NA> GLU B 161 <NA> 7.889 -3.222 23.448  
## 2890 ATOM 2891 CB <NA> GLU B 161 <NA> 6.947 -4.953 26.062  
## 2891 ATOM 2892 CG <NA> GLU B 161 <NA> 7.820 -3.872 26.697  
## 2892 ATOM 2893 CD <NA> GLU B 161 <NA> 7.970 -4.043 28.202  
## 2893 ATOM 2894 OE1 <NA> GLU B 161 <NA> 6.958 -4.275 28.891  
## 2894 ATOM 2895 OE2 <NA> GLU B 161 <NA> 9.098 -3.921 28.713  
## 2895 ATOM 2896 N <NA> GLU B 162 <NA> 8.075 -5.419 23.076  
## 2896 ATOM 2897 CA <NA> GLU B 162 <NA> 9.161 -5.223 22.116  
## 2897 ATOM 2898 C <NA> GLU B 162 <NA> 8.631 -4.510 20.871  
## 2898 ATOM 2899 O <NA> GLU B 162 <NA> 9.131 -3.451 20.484  
## 2899 ATOM 2900 CB <NA> GLU B 162 <NA> 9.791 -6.557 21.709  
## 2900 ATOM 2901 CG <NA> GLU B 162 <NA> 10.879 -6.397 20.633  
## 2901 ATOM 2902 CD <NA> GLU B 162 <NA> 11.432 -7.721 20.114  
## 2902 ATOM 2903 OE1 <NA> GLU B 162 <NA> 10.642 -8.683 19.946  
## 2903 ATOM 2904 OE2 <NA> GLU B 162 <NA> 12.660 -7.790 19.867  
## 2904 ATOM 2905 N <NA> THR B 163 <NA> 7.612 -5.098 20.255  
## 2905 ATOM 2906 CA <NA> THR B 163 <NA> 7.007 -4.533 19.068  
## 2906 ATOM 2907 C <NA> THR B 163 <NA> 6.532 -3.112 19.336  
## 2907 ATOM 2908 O <NA> THR B 163 <NA> 6.780 -2.224 18.521  
## 2908 ATOM 2909 CB <NA> THR B 163 <NA> 5.842 -5.398 18.604  
## 2909 ATOM 2910 OG1 <NA> THR B 163 <NA> 6.271 -6.765 18.551  
## 2910 ATOM 2911 CG2 <NA> THR B 163 <NA> 5.389 -4.976 17.227  
## 2911 ATOM 2912 N <NA> VAL B 164 <NA> 5.912 -2.888 20.500  
## 2912 ATOM 2913 CA <NA> VAL B 164 <NA> 5.415 -1.563 20.887  
## 2913 ATOM 2914 C <NA> VAL B 164 <NA> 6.572 -0.587 21.006  
## 2914 ATOM 2915 O <NA> VAL B 164 <NA> 6.503 0.521 20.503  
## 2915 ATOM 2916 CB <NA> VAL B 164 <NA> 4.628 -1.592 22.224  
## 2916 ATOM 2917 CG1 <NA> VAL B 164 <NA> 4.325 -0.167 22.728  
## 2917 ATOM 2918 CG2 <NA> VAL B 164 <NA> 3.349 -2.383 22.048  
## 2918 ATOM 2919 N <NA> ARG B 165 <NA> 7.665 -1.002 21.614  
## 2919 ATOM 2920 CA <NA> ARG B 165 <NA> 8.769 -0.089 21.751  
## 2920 ATOM 2921 C <NA> ARG B 165 <NA> 9.453 0.225 20.443  
## 2921 ATOM 2922 O <NA> ARG B 165 <NA> 10.041 1.290 20.300  
## 2922 ATOM 2923 CB <NA> ARG B 165 <NA> 9.748 -0.590 22.781  
## 2923 ATOM 2924 CG <NA> ARG B 165 <NA> 9.190 -0.500 24.169  
## 2924 ATOM 2925 CD <NA> ARG B 165 <NA> 10.328 -0.420 25.154  
## 2925 ATOM 2926 NE <NA> ARG B 165 <NA> 9.968 0.411 26.296  
## 2926 ATOM 2927 CZ <NA> ARG B 165 <NA> 9.516 -0.069 27.445  
## 2927 ATOM 2928 NH1 <NA> ARG B 165 <NA> 9.379 -1.377 27.607  
## 2928 ATOM 2929 NH2 <NA> ARG B 165 <NA> 9.213 0.755 28.428  
## 2929 ATOM 2930 N <NA> LYS B 166 <NA> 9.355 -0.669 19.473  
## 2930 ATOM 2931 CA <NA> LYS B 166 <NA> 9.965 -0.408 18.172  
## 2931 ATOM 2932 C <NA> LYS B 166 <NA> 9.146 0.615 17.399  
## 2932 ATOM 2933 O <NA> LYS B 166 <NA> 9.703 1.541 16.808  
## 2933 ATOM 2934 CB <NA> LYS B 166 <NA> 10.124 -1.693 17.368  
## 2934 ATOM 2935 CG <NA> LYS B 166 <NA> 11.374 -2.466 17.725  
## 2935 ATOM 2936 CD <NA> LYS B 166 <NA> 11.374 -3.855 17.096  
## 2936 ATOM 2937 CE <NA> LYS B 166 <NA> 10.211 -4.700 17.615  
## 2937 ATOM 2938 NZ <NA> LYS B 166 <NA> 10.239 -6.122 17.153  
## 2938 ATOM 2939 N <NA> ARG B 167 <NA> 7.826 0.448 17.388  
## 2939 ATOM 2940 CA <NA> ARG B 167 <NA> 6.950 1.400 16.710  
## 2940 ATOM 2941 C <NA> ARG B 167 <NA> 7.256 2.814 17.207  
## 2941 ATOM 2942 O <NA> ARG B 167 <NA> 7.372 3.747 16.416  
## 2942 ATOM 2943 CB <NA> ARG B 167 <NA> 5.484 1.123 17.025  
## 2943 ATOM 2944 CG <NA> ARG B 167 <NA> 4.788 0.213 16.089  
## 2944 ATOM 2945 CD <NA> ARG B 167 <NA> 3.287 0.435 16.182  
## 2945 ATOM 2946 NE <NA> ARG B 167 <NA> 2.728 0.178 17.511  
## 2946 ATOM 2947 CZ <NA> ARG B 167 <NA> 2.169 -0.975 17.884  
## 2947 ATOM 2948 NH1 <NA> ARG B 167 <NA> 2.118 -2.007 17.048  
## 2948 ATOM 2949 NH2 <NA> ARG B 167 <NA> 1.679 -1.109 19.107  
## 2949 ATOM 2950 N <NA> LEU B 168 <NA> 7.373 2.962 18.525  
## 2950 ATOM 2951 CA <NA> LEU B 168 <NA> 7.634 4.258 19.121  
## 2951 ATOM 2952 C <NA> LEU B 168 <NA> 8.937 4.867 18.675  
## 2952 ATOM 2953 O <NA> LEU B 168 <NA> 8.945 6.015 18.249  
## 2953 ATOM 2954 CB <NA> LEU B 168 <NA> 7.553 4.210 20.652  
## 2954 ATOM 2955 CG <NA> LEU B 168 <NA> 6.179 3.898 21.281  
## 2955 ATOM 2956 CD1 <NA> LEU B 168 <NA> 6.318 3.725 22.786  
## 2956 ATOM 2957 CD2 <NA> LEU B 168 <NA> 5.130 4.958 20.956  
## 2957 ATOM 2958 N <NA> VAL B 169 <NA> 10.038 4.129 18.748  
## 2958 ATOM 2959 CA <NA> VAL B 169 <NA> 11.300 4.722 18.321  
## 2959 ATOM 2960 C <NA> VAL B 169 <NA> 11.197 5.196 16.891  
## 2960 ATOM 2961 O <NA> VAL B 169 <NA> 11.543 6.336 16.581  
## 2961 ATOM 2962 CB <NA> VAL B 169 <NA> 12.505 3.770 18.454  
## 2962 ATOM 2963 CG1 <NA> VAL B 169 <NA> 12.625 3.306 19.878  
## 2963 ATOM 2964 CG2 <NA> VAL B 169 <NA> 12.394 2.606 17.482  
## 2964 ATOM 2965 N <NA> GLU B 170 <NA> 10.644 4.343 16.043  
## 2965 ATOM 2966 CA <NA> GLU B 170 <NA> 10.481 4.671 14.649  
## 2966 ATOM 2967 C <NA> GLU B 170 <NA> 9.649 5.926 14.506  
## 2967 ATOM 2968 O <NA> GLU B 170 <NA> 10.026 6.869 13.819  
## 2968 ATOM 2969 CB <NA> GLU B 170 <NA> 9.824 3.520 13.909  
## 2969 ATOM 2970 CG <NA> GLU B 170 <NA> 9.437 3.874 12.486  
## 2970 ATOM 2971 CD <NA> GLU B 170 <NA> 9.475 2.680 11.545  
## 2971 ATOM 2972 OE1 <NA> GLU B 170 <NA> 9.280 1.533 12.020  
## 2972 ATOM 2973 OE2 <NA> GLU B 170 <NA> 9.708 2.901 10.328  
## 2973 ATOM 2974 N <NA> TYR B 171 <NA> 8.536 5.962 15.208  
## 2974 ATOM 2975 CA <NA> TYR B 171 <NA> 7.671 7.107 15.142  
## 2975 ATOM 2976 C <NA> TYR B 171 <NA> 8.419 8.368 15.549  
## 2976 ATOM 2977 O <NA> TYR B 171 <NA> 8.351 9.396 14.881  
## 2977 ATOM 2978 CB <NA> TYR B 171 <NA> 6.463 6.898 16.049  
## 2978 ATOM 2979 CG <NA> TYR B 171 <NA> 5.679 8.157 16.252  
## 2979 ATOM 2980 CD1 <NA> TYR B 171 <NA> 4.660 8.518 15.363  
## 2980 ATOM 2981 CD2 <NA> TYR B 171 <NA> 6.003 9.035 17.291  
## 2981 ATOM 2982 CE1 <NA> TYR B 171 <NA> 3.996 9.722 15.505  
## 2982 ATOM 2983 CE2 <NA> TYR B 171 <NA> 5.358 10.233 17.434  
## 2983 ATOM 2984 CZ <NA> TYR B 171 <NA> 4.353 10.576 16.534  
## 2984 ATOM 2985 OH <NA> TYR B 171 <NA> 3.744 11.804 16.653  
## 2985 ATOM 2986 N <NA> HIS B 172 <NA> 9.137 8.307 16.650  
## 2986 ATOM 2987 CA <NA> HIS B 172 <NA> 9.845 9.492 17.107  
## 2987 ATOM 2988 C <NA> HIS B 172 <NA> 10.962 10.013 16.213  
## 2988 ATOM 2989 O <NA> HIS B 172 <NA> 11.125 11.232 16.078  
## 2989 ATOM 2990 CB <NA> HIS B 172 <NA> 10.368 9.286 18.518  
## 2990 ATOM 2991 CG <NA> HIS B 172 <NA> 9.308 9.373 19.563  
## 2991 ATOM 2992 ND1 <NA> HIS B 172 <NA> 8.552 10.508 19.760  
## 2992 ATOM 2993 CD2 <NA> HIS B 172 <NA> 8.886 8.472 20.482  
## 2993 ATOM 2994 CE1 <NA> HIS B 172 <NA> 7.710 10.305 20.757  
## 2994 ATOM 2995 NE2 <NA> HIS B 172 <NA> 7.892 9.076 21.211  
## 2995 ATOM 2996 N <NA> GLN B 173 <NA> 11.750 9.119 15.626  
## 2996 ATOM 2997 CA <NA> GLN B 173 <NA> 12.834 9.573 14.771  
## 2997 ATOM 2998 C <NA> GLN B 173 <NA> 12.288 10.218 13.500  
## 2998 ATOM 2999 O <NA> GLN B 173 <NA> 12.900 11.137 12.954  
## 2999 ATOM 3000 CB <NA> GLN B 173 <NA> 13.820 8.441 14.476  
## 3000 ATOM 3001 CG <NA> GLN B 173 <NA> 13.238 7.216 13.815  
## 3001 ATOM 3002 CD <NA> GLN B 173 <NA> 14.182 6.014 13.891  
## 3002 ATOM 3003 OE1 <NA> GLN B 173 <NA> 14.961 5.881 14.843  
## 3003 ATOM 3004 NE2 <NA> GLN B 173 <NA> 14.106 5.127 12.898  
## 3004 ATOM 3005 N <NA> MET B 174 <NA> 11.106 9.761 13.082  
## 3005 ATOM 3006 CA <NA> MET B 174 <NA> 10.379 10.266 11.907  
## 3006 ATOM 3007 C <NA> MET B 174 <NA> 9.679 11.620 12.182  
## 3007 ATOM 3008 O <NA> MET B 174 <NA> 9.686 12.528 11.348  
## 3008 ATOM 3009 CB <NA> MET B 174 <NA> 9.260 9.285 11.533  
## 3009 ATOM 3010 CG <NA> MET B 174 <NA> 9.520 8.251 10.457  
## 3010 ATOM 3011 SD <NA> MET B 174 <NA> 7.994 8.032 9.423  
## 3011 ATOM 3012 CE <NA> MET B 174 <NA> 6.557 8.311 10.630  
## 3012 ATOM 3013 N <NA> THR B 175 <NA> 9.093 11.742 13.365  
## 3013 ATOM 3014 CA <NA> THR B 175 <NA> 8.326 12.914 13.747  
## 3014 ATOM 3015 C <NA> THR B 175 <NA> 9.052 14.073 14.412  
## 3015 ATOM 3016 O <NA> THR B 175 <NA> 8.547 15.205 14.446  
## 3016 ATOM 3017 CB <NA> THR B 175 <NA> 7.169 12.459 14.634  
## 3017 ATOM 3018 OG1 <NA> THR B 175 <NA> 6.476 11.403 13.963  
## 3018 ATOM 3019 CG2 <NA> THR B 175 <NA> 6.191 13.581 14.888  
## 3019 ATOM 3020 N <NA> ALA B 176 <NA> 10.206 13.798 14.994  
## 3020 ATOM 3021 CA <NA> ALA B 176 <NA> 10.967 14.848 15.655  
## 3021 ATOM 3022 C <NA> ALA B 176 <NA> 11.228 16.090 14.791  
## 3022 ATOM 3023 O <NA> ALA B 176 <NA> 10.912 17.206 15.211  
## 3023 ATOM 3024 CB <NA> ALA B 176 <NA> 12.269 14.283 16.202  
## 3024 ATOM 3025 N <NA> PRO B 177 <NA> 11.825 15.932 13.587  
## 3025 ATOM 3026 CA <NA> PRO B 177 <NA> 12.066 17.135 12.772  
## 3026 ATOM 3027 C <NA> PRO B 177 <NA> 10.798 17.838 12.291  
## 3027 ATOM 3028 O <NA> PRO B 177 <NA> 10.769 19.072 12.222  
## 3028 ATOM 3029 CB <NA> PRO B 177 <NA> 12.941 16.626 11.627  
## 3029 ATOM 3030 CG <NA> PRO B 177 <NA> 12.613 15.185 11.535  
## 3030 ATOM 3031 CD <NA> PRO B 177 <NA> 12.428 14.744 12.960  
## 3031 ATOM 3032 N <NA> LEU B 178 <NA> 9.730 17.067 12.055  
## 3032 ATOM 3033 CA <NA> LEU B 178 <NA> 8.442 17.629 11.630  
## 3033 ATOM 3034 C <NA> LEU B 178 <NA> 7.919 18.540 12.733  
## 3034 ATOM 3035 O <NA> LEU B 178 <NA> 7.424 19.638 12.474  
## 3035 ATOM 3036 CB <NA> LEU B 178 <NA> 7.422 16.527 11.332  
## 3036 ATOM 3037 CG <NA> LEU B 178 <NA> 6.116 17.022 10.693  
## 3037 ATOM 3038 CD1 <NA> LEU B 178 <NA> 6.382 17.463 9.293  
## 3038 ATOM 3039 CD2 <NA> LEU B 178 <NA> 5.109 15.949 10.669  
## 3039 ATOM 3040 N <NA> ILE B 179 <NA> 8.079 18.096 13.976  
## 3040 ATOM 3041 CA <NA> ILE B 179 <NA> 7.661 18.886 15.121  
## 3041 ATOM 3042 C <NA> ILE B 179 <NA> 8.466 20.170 15.108  
## 3042 ATOM 3043 O <NA> ILE B 179 <NA> 7.916 21.241 15.353  
## 3043 ATOM 3044 CB <NA> ILE B 179 <NA> 7.945 18.168 16.458  
## 3044 ATOM 3045 CG1 <NA> ILE B 179 <NA> 7.191 16.852 16.519  
## 3045 ATOM 3046 CG2 <NA> ILE B 179 <NA> 7.544 19.059 17.636  
## 3046 ATOM 3047 CD1 <NA> ILE B 179 <NA> 5.712 17.015 16.264  
## 3047 ATOM 3048 N <NA> GLY B 180 <NA> 9.773 20.056 14.850  
## 3048 ATOM 3049 CA <NA> GLY B 180 <NA> 10.631 21.229 14.807  
## 3049 ATOM 3050 C <NA> GLY B 180 <NA> 10.255 22.129 13.638  
## 3050 ATOM 3051 O <NA> GLY B 180 <NA> 10.285 23.345 13.714  
## 3051 ATOM 3052 N <NA> TYR B 181 <NA> 9.867 21.508 12.542  
## 3052 ATOM 3053 CA <NA> TYR B 181 <NA> 9.441 22.239 11.366  
## 3053 ATOM 3054 C <NA> TYR B 181 <NA> 8.232 23.108 11.730  
## 3054 ATOM 3055 O <NA> TYR B 181 <NA> 8.215 24.315 11.432  
## 3055 ATOM 3056 CB <NA> TYR B 181 <NA> 9.076 21.232 10.252  
## 3056 ATOM 3057 CG <NA> TYR B 181 <NA> 8.339 21.830 9.060  
## 3057 ATOM 3058 CD1 <NA> TYR B 181 <NA> 6.944 21.952 9.057  
## 3058 ATOM 3059 CD2 <NA> TYR B 181 <NA> 9.027 22.271 7.945  
## 3059 ATOM 3060 CE1 <NA> TYR B 181 <NA> 6.265 22.496 7.988  
## 3060 ATOM 3061 CE2 <NA> TYR B 181 <NA> 8.344 22.818 6.856  
## 3061 ATOM 3062 CZ <NA> TYR B 181 <NA> 6.966 22.928 6.890  
## 3062 ATOM 3063 OH <NA> TYR B 181 <NA> 6.307 23.476 5.812  
## 3063 ATOM 3064 N <NA> TYR B 182 <NA> 7.225 22.499 12.370  
## 3064 ATOM 3065 CA <NA> TYR B 182 <NA> 6.006 23.222 12.754  
## 3065 ATOM 3066 C <NA> TYR B 182 <NA> 6.204 24.295 13.783  
## 3066 ATOM 3067 O <NA> TYR B 182 <NA> 5.678 25.400 13.617  
## 3067 ATOM 3068 CB <NA> TYR B 182 <NA> 4.863 22.273 13.152  
## 3068 ATOM 3069 CG <NA> TYR B 182 <NA> 4.171 21.707 11.934  
## 3069 ATOM 3070 CD1 <NA> TYR B 182 <NA> 3.792 22.556 10.878  
## 3070 ATOM 3071 CD2 <NA> TYR B 182 <NA> 3.948 20.336 11.791  
## 3071 ATOM 3072 CE1 <NA> TYR B 182 <NA> 3.207 22.048 9.691  
## 3072 ATOM 3073 CE2 <NA> TYR B 182 <NA> 3.353 19.807 10.612  
## 3073 ATOM 3074 CZ <NA> TYR B 182 <NA> 2.992 20.676 9.573  
## 3074 ATOM 3075 OH <NA> TYR B 182 <NA> 2.419 20.195 8.412  
## 3075 ATOM 3076 N <NA> SER B 183 <NA> 7.000 24.023 14.812  
## 3076 ATOM 3077 CA <NA> SER B 183 <NA> 7.256 25.033 15.847  
## 3077 ATOM 3078 C <NA> SER B 183 <NA> 7.813 26.293 15.211  
## 3078 ATOM 3079 O <NA> SER B 183 <NA> 7.462 27.395 15.626  
## 3079 ATOM 3080 CB <NA> SER B 183 <NA> 8.253 24.526 16.895  
## 3080 ATOM 3081 OG <NA> SER B 183 <NA> 7.913 23.226 17.331  
## 3081 ATOM 3082 N <NA> LYS B 184 <NA> 8.665 26.138 14.194  
## 3082 ATOM 3083 CA <NA> LYS B 184 <NA> 9.241 27.303 13.525  
## 3083 ATOM 3084 C <NA> LYS B 184 <NA> 8.234 27.949 12.605  
## 3084 ATOM 3085 O <NA> LYS B 184 <NA> 8.256 29.161 12.437  
## 3085 ATOM 3086 CB <NA> LYS B 184 <NA> 10.521 26.965 12.756  
## 3086 ATOM 3087 CG <NA> LYS B 184 <NA> 11.783 26.869 13.613  
## 3087 ATOM 3088 CD <NA> LYS B 184 <NA> 13.009 26.648 12.726  
## 3088 ATOM 3089 CE <NA> LYS B 184 <NA> 14.335 26.682 13.498  
## 3089 ATOM 3090 NZ <NA> LYS B 184 <NA> 15.514 26.360 12.611  
## 3090 ATOM 3091 N <NA> GLU B 185 <NA> 7.378 27.149 11.976  
## 3091 ATOM 3092 CA <NA> GLU B 185 <NA> 6.350 27.713 11.107  
## 3092 ATOM 3093 C <NA> GLU B 185 <NA> 5.538 28.651 11.962  
## 3093 ATOM 3094 O <NA> GLU B 185 <NA> 5.174 29.751 11.531  
## 3094 ATOM 3095 CB <NA> GLU B 185 <NA> 5.438 26.631 10.584  
## 3095 ATOM 3096 CG <NA> GLU B 185 <NA> 6.019 25.850 9.449  
## 3096 ATOM 3097 CD <NA> GLU B 185 <NA> 6.205 26.708 8.223  
## 3097 ATOM 3098 OE1 <NA> GLU B 185 <NA> 5.194 27.141 7.628  
## 3098 ATOM 3099 OE2 <NA> GLU B 185 <NA> 7.369 26.965 7.868  
## 3099 ATOM 3100 N <NA> ALA B 186 <NA> 5.301 28.208 13.194  
## 3100 ATOM 3101 CA <NA> ALA B 186 <NA> 4.548 28.948 14.195  
## 3101 ATOM 3102 C <NA> ALA B 186 <NA> 5.273 30.224 14.595  
## 3102 ATOM 3103 O <NA> ALA B 186 <NA> 4.651 31.282 14.692  
## 3103 ATOM 3104 CB <NA> ALA B 186 <NA> 4.306 28.081 15.392  
## 3104 ATOM 3105 N <NA> GLU B 187 <NA> 6.582 30.125 14.839  
## 3105 ATOM 3106 CA <NA> GLU B 187 <NA> 7.408 31.289 15.194  
## 3106 ATOM 3107 C <NA> GLU B 187 <NA> 7.348 32.264 14.033  
## 3107 ATOM 3108 O <NA> GLU B 187 <NA> 7.400 33.473 14.219  
## 3108 ATOM 3109 CB <NA> GLU B 187 <NA> 8.880 30.895 15.382  
## 3109 ATOM 3110 CG <NA> GLU B 187 <NA> 9.297 30.386 16.765  
## 3110 ATOM 3111 CD <NA> GLU B 187 <NA> 10.793 29.999 16.840  
## 3111 ATOM 3112 OE1 <NA> GLU B 187 <NA> 11.611 30.582 16.083  
## 3112 ATOM 3113 OE2 <NA> GLU B 187 <NA> 11.149 29.110 17.655  
## 3113 ATOM 3114 N <NA> ALA B 188 <NA> 7.319 31.706 12.830  
## 3114 ATOM 3115 CA <NA> ALA B 188 <NA> 7.250 32.468 11.595  
## 3115 ATOM 3116 C <NA> ALA B 188 <NA> 5.885 33.123 11.517  
## 3116 ATOM 3117 O <NA> ALA B 188 <NA> 5.715 34.155 10.887  
## 3117 ATOM 3118 CB <NA> ALA B 188 <NA> 7.454 31.535 10.406  
## 3118 ATOM 3119 N <NA> GLY B 189 <NA> 4.898 32.486 12.132  
## 3119 ATOM 3120 CA <NA> GLY B 189 <NA> 3.554 33.032 12.140  
## 3120 ATOM 3121 C <NA> GLY B 189 <NA> 2.631 32.446 11.106  
## 3121 ATOM 3122 O <NA> GLY B 189 <NA> 1.503 32.904 10.970  
## 3122 ATOM 3123 N <NA> ASN B 190 <NA> 3.063 31.380 10.440  
## 3123 ATOM 3124 CA <NA> ASN B 190 <NA> 2.244 30.752 9.408  
## 3124 ATOM 3125 C <NA> ASN B 190 <NA> 1.166 29.788 9.924  
## 3125 ATOM 3126 O <NA> ASN B 190 <NA> 0.235 29.435 9.202  
## 3126 ATOM 3127 CB <NA> ASN B 190 <NA> 3.140 30.065 8.375  
## 3127 ATOM 3128 CG <NA> ASN B 190 <NA> 4.140 31.016 7.747  
## 3128 ATOM 3129 OD1 <NA> ASN B 190 <NA> 3.886 32.216 7.642  
## 3129 ATOM 3130 ND2 <NA> ASN B 190 <NA> 5.294 30.493 7.352  
## 3130 ATOM 3131 N <NA> THR B 191 <NA> 1.279 29.387 11.182  
## 3131 ATOM 3132 CA <NA> THR B 191 <NA> 0.322 28.473 11.791  
## 3132 ATOM 3133 C <NA> THR B 191 <NA> 0.539 28.581 13.305  
## 3133 ATOM 3134 O <NA> THR B 191 <NA> 1.345 29.390 13.752  
## 3134 ATOM 3135 CB <NA> THR B 191 <NA> 0.561 27.024 11.285  
## 3135 ATOM 3136 OG1 <NA> THR B 191 <NA> -0.542 26.176 11.639  
## 3136 ATOM 3137 CG2 <NA> THR B 191 <NA> 1.834 26.458 11.875  
## 3137 ATOM 3138 N <NA> LYS B 192 <NA> -0.262 27.882 14.098  
## 3138 ATOM 3139 CA <NA> LYS B 192 <NA> -0.093 27.886 15.554  
## 3139 ATOM 3140 C <NA> LYS B 192 <NA> 0.147 26.426 15.907  
## 3140 ATOM 3141 O <NA> LYS B 192 <NA> -0.481 25.543 15.358  
## 3141 ATOM 3142 CB <NA> LYS B 192 <NA> -1.331 28.413 16.282  
## 3142 ATOM 3143 CG <NA> LYS B 192 <NA> -1.465 29.918 16.315  
## 3143 ATOM 3144 CD <NA> LYS B 192 <NA> -2.097 30.466 15.041  
## 3144 ATOM 3145 CE <NA> LYS B 192 <NA> -3.618 30.223 14.985  
## 3145 ATOM 3146 NZ <NA> LYS B 192 <NA> -4.220 30.572 13.655  
## 3146 ATOM 3147 N <NA> TYR B 193 <NA> 1.077 26.170 16.803  
## 3147 ATOM 3148 CA <NA> TYR B 193 <NA> 1.420 24.810 17.171  
## 3148 ATOM 3149 C <NA> TYR B 193 <NA> 1.173 24.654 18.665  
## 3149 ATOM 3150 O <NA> TYR B 193 <NA> 1.429 25.569 19.434  
## 3150 ATOM 3151 CB <NA> TYR B 193 <NA> 2.889 24.572 16.781  
## 3151 ATOM 3152 CG <NA> TYR B 193 <NA> 3.504 23.378 17.421  
## 3152 ATOM 3153 CD1 <NA> TYR B 193 <NA> 3.299 22.101 16.913  
## 3153 ATOM 3154 CD2 <NA> TYR B 193 <NA> 4.186 23.510 18.619  
## 3154 ATOM 3155 CE1 <NA> TYR B 193 <NA> 3.747 20.988 17.601  
## 3155 ATOM 3156 CE2 <NA> TYR B 193 <NA> 4.628 22.413 19.312  
## 3156 ATOM 3157 CZ <NA> TYR B 193 <NA> 4.408 21.164 18.812  
## 3157 ATOM 3158 OH <NA> TYR B 193 <NA> 4.826 20.099 19.571  
## 3158 ATOM 3159 N <NA> ALA B 194 <NA> 0.619 23.526 19.094  
## 3159 ATOM 3160 CA <NA> ALA B 194 <NA> 0.379 23.348 20.512  
## 3160 ATOM 3161 C <NA> ALA B 194 <NA> 0.559 21.915 20.968  
## 3161 ATOM 3162 O <NA> ALA B 194 <NA> 0.146 20.984 20.300  
## 3162 ATOM 3163 CB <NA> ALA B 194 <NA> -1.013 23.855 20.885  
## 3163 ATOM 3164 N <NA> LYS B 195 <NA> 1.231 21.745 22.097  
## 3164 ATOM 3165 CA <NA> LYS B 195 <NA> 1.450 20.421 22.664  
## 3165 ATOM 3166 C <NA> LYS B 195 <NA> 0.302 20.249 23.657  
## 3166 ATOM 3167 O <NA> LYS B 195 <NA> -0.086 21.205 24.336  
## 3167 ATOM 3168 CB <NA> LYS B 195 <NA> 2.790 20.385 23.388  
## 3168 ATOM 3169 CG <NA> LYS B 195 <NA> 3.225 19.012 23.836  
## 3169 ATOM 3170 CD <NA> LYS B 195 <NA> 4.356 18.517 22.964  
## 3170 ATOM 3171 CE <NA> LYS B 195 <NA> 5.534 19.493 22.948  
## 3171 ATOM 3172 NZ <NA> LYS B 195 <NA> 6.666 19.045 22.064  
## 3172 ATOM 3173 N <NA> VAL B 196 <NA> -0.256 19.050 23.726  
## 3173 ATOM 3174 CA <NA> VAL B 196 <NA> -1.378 18.782 24.608  
## 3174 ATOM 3175 C <NA> VAL B 196 <NA> -0.951 17.624 25.493  
## 3175 ATOM 3176 O <NA> VAL B 196 <NA> -0.577 16.572 24.993  
## 3176 ATOM 3177 CB <NA> VAL B 196 <NA> -2.677 18.414 23.772  
## 3177 ATOM 3178 CG1 <NA> VAL B 196 <NA> -3.800 17.974 24.666  
## 3178 ATOM 3179 CG2 <NA> VAL B 196 <NA> -3.138 19.605 22.950  
## 3179 ATOM 3180 N <NA> ASP B 197 <NA> -0.897 17.866 26.799  
## 3180 ATOM 3181 CA <NA> ASP B 197 <NA> -0.536 16.847 27.785  
## 3181 ATOM 3182 C <NA> ASP B 197 <NA> -1.742 15.902 27.827  
## 3182 ATOM 3183 O <NA> ASP B 197 <NA> -2.793 16.246 28.361  
## 3183 ATOM 3184 CB <NA> ASP B 197 <NA> -0.336 17.519 29.143  
## 3184 ATOM 3185 CG <NA> ASP B 197 <NA> -0.013 16.544 30.253  
## 3185 ATOM 3186 OD1 <NA> ASP B 197 <NA> 0.162 15.336 30.000  
## 3186 ATOM 3187 OD2 <NA> ASP B 197 <NA> 0.071 17.012 31.403  
## 3187 ATOM 3188 N <NA> GLY B 198 <NA> -1.585 14.732 27.226  
## 3188 ATOM 3189 CA <NA> GLY B 198 <NA> -2.666 13.775 27.161  
## 3189 ATOM 3190 C <NA> GLY B 198 <NA> -2.662 12.792 28.290  
## 3190 ATOM 3191 O <NA> GLY B 198 <NA> -3.199 11.689 28.174  
## 3191 ATOM 3192 N <NA> THR B 199 <NA> -1.983 13.150 29.369  
## 3192 ATOM 3193 CA <NA> THR B 199 <NA> -1.951 12.283 30.540  
## 3193 ATOM 3194 C <NA> THR B 199 <NA> -3.123 12.730 31.426  
## 3194 ATOM 3195 O <NA> THR B 199 <NA> -3.674 11.944 32.192  
## 3195 ATOM 3196 CB <NA> THR B 199 <NA> -0.602 12.384 31.263  
## 3196 ATOM 3197 OG1 <NA> THR B 199 <NA> -0.419 13.717 31.744  
## 3197 ATOM 3198 CG2 <NA> THR B 199 <NA> 0.534 12.066 30.287  
## 3198 ATOM 3199 N <NA> LYS B 200 <NA> -3.567 13.970 31.227  
## 3199 ATOM 3200 CA <NA> LYS B 200 <NA> -4.673 14.521 31.984  
## 3200 ATOM 3201 C <NA> LYS B 200 <NA> -5.985 13.806 31.751  
## 3201 ATOM 3202 O <NA> LYS B 200 <NA> -6.129 13.018 30.816  
## 3202 ATOM 3203 CB <NA> LYS B 200 <NA> -4.886 15.981 31.639  
## 3203 ATOM 3204 CG <NA> LYS B 200 <NA> -3.738 16.843 31.990  
## 3204 ATOM 3205 CD <NA> LYS B 200 <NA> -4.006 18.260 31.550  
## 3205 ATOM 3206 CE <NA> LYS B 200 <NA> -2.827 19.130 31.853  
## 3206 ATOM 3207 NZ <NA> LYS B 200 <NA> -3.163 20.545 31.604  
## 3207 ATOM 3208 N <NA> PRO B 201 <NA> -6.921 13.971 32.698  
## 3208 ATOM 3209 CA <NA> PRO B 201 <NA> -8.222 13.333 32.534  
## 3209 ATOM 3210 C <NA> PRO B 201 <NA> -8.877 13.979 31.304  
## 3210 ATOM 3211 O <NA> PRO B 201 <NA> -8.731 15.192 31.062  
## 3211 ATOM 3212 CB <NA> PRO B 201 <NA> -8.945 13.685 33.849  
## 3212 ATOM 3213 CG <NA> PRO B 201 <NA> -8.169 14.853 34.418  
## 3213 ATOM 3214 CD <NA> PRO B 201 <NA> -6.769 14.507 34.065  
## 3214 ATOM 3215 N <NA> VAL B 202 <NA> -9.594 13.162 30.541  
## 3215 ATOM 3216 CA <NA> VAL B 202 <NA> -10.246 13.601 29.317  
## 3216 ATOM 3217 C <NA> VAL B 202 <NA> -10.991 14.919 29.392  
## 3217 ATOM 3218 O <NA> VAL B 202 <NA> -10.954 15.708 28.444  
## 3218 ATOM 3219 CB <NA> VAL B 202 <NA> -11.183 12.543 28.771  
## 3219 ATOM 3220 CG1 <NA> VAL B 202 <NA> -11.817 13.034 27.489  
## 3220 ATOM 3221 CG2 <NA> VAL B 202 <NA> -10.418 11.269 28.508  
## 3221 ATOM 3222 N <NA> ALA B 203 <NA> -11.649 15.165 30.514  
## 3222 ATOM 3223 CA <NA> ALA B 203 <NA> -12.398 16.399 30.686  
## 3223 ATOM 3224 C <NA> ALA B 203 <NA> -11.482 17.581 30.760  
## 3224 ATOM 3225 O <NA> ALA B 203 <NA> -11.900 18.693 30.423  
## 3225 ATOM 3226 CB <NA> ALA B 203 <NA> -13.237 16.336 31.925  
## 3226 ATOM 3227 N <NA> GLU B 204 <NA> -10.247 17.357 31.228  
## 3227 ATOM 3228 CA <NA> GLU B 204 <NA> -9.272 18.444 31.336  
## 3228 ATOM 3229 C <NA> GLU B 204 <NA> -8.560 18.711 30.025  
## 3229 ATOM 3230 O <NA> GLU B 204 <NA> -8.200 19.857 29.743  
## 3230 ATOM 3231 CB <NA> GLU B 204 <NA> -8.262 18.212 32.439  
## 3231 ATOM 3232 CG <NA> GLU B 204 <NA> -7.841 19.519 33.091  
## 3232 ATOM 3233 CD <NA> GLU B 204 <NA> -6.695 19.348 34.076  
## 3233 ATOM 3234 OE1 <NA> GLU B 204 <NA> -6.637 18.310 34.785  
## 3234 ATOM 3235 OE2 <NA> GLU B 204 <NA> -5.836 20.258 34.133  
## 3235 ATOM 3236 N <NA> VAL B 205 <NA> -8.370 17.661 29.223  
## 3236 ATOM 3237 CA <NA> VAL B 205 <NA> -7.762 17.807 27.900  
## 3237 ATOM 3238 C <NA> VAL B 205 <NA> -8.738 18.649 27.074  
## 3238 ATOM 3239 O <NA> VAL B 205 <NA> -8.374 19.640 26.445  
## 3239 ATOM 3240 CB <NA> VAL B 205 <NA> -7.587 16.449 27.178  
## 3240 ATOM 3241 CG1 <NA> VAL B 205 <NA> -6.943 16.660 25.821  
## 3241 ATOM 3242 CG2 <NA> VAL B 205 <NA> -6.742 15.502 28.004  
## 3242 ATOM 3243 N <NA> ARG B 206 <NA> -9.998 18.259 27.117  
## 3243 ATOM 3244 CA <NA> ARG B 206 <NA> -11.060 18.959 26.410  
## 3244 ATOM 3245 C <NA> ARG B 206 <NA> -11.081 20.463 26.794  
## 3245 ATOM 3246 O <NA> ARG B 206 <NA> -11.120 21.341 25.923  
## 3246 ATOM 3247 CB <NA> ARG B 206 <NA> -12.351 18.236 26.744  
## 3247 ATOM 3248 CG <NA> ARG B 206 <NA> -13.571 18.637 26.019  
## 3248 ATOM 3249 CD <NA> ARG B 206 <NA> -14.664 17.656 26.437  
## 3249 ATOM 3250 NE <NA> ARG B 206 <NA> -16.010 18.074 26.062  
## 3250 ATOM 3251 CZ <NA> ARG B 206 <NA> -16.593 19.198 26.478  
## 3251 ATOM 3252 NH1 <NA> ARG B 206 <NA> -15.947 20.043 27.278  
## 3252 ATOM 3253 NH2 <NA> ARG B 206 <NA> -17.827 19.483 26.082  
## 3253 ATOM 3254 N <NA> ALA B 207 <NA> -10.983 20.768 28.088  
## 3254 ATOM 3255 CA <NA> ALA B 207 <NA> -10.960 22.155 28.533  
## 3255 ATOM 3256 C <NA> ALA B 207 <NA> -9.707 22.826 27.983  
## 3256 ATOM 3257 O <NA> ALA B 207 <NA> -9.742 24.005 27.628  
## 3257 ATOM 3258 CB <NA> ALA B 207 <NA> -10.962 22.233 30.037  
## 3258 ATOM 3259 N <NA> ASP B 208 <NA> -8.595 22.089 27.944  
## 3259 ATOM 3260 CA <NA> ASP B 208 <NA> -7.347 22.628 27.402  
## 3260 ATOM 3261 C <NA> ASP B 208 <NA> -7.523 22.999 25.925  
## 3261 ATOM 3262 O <NA> ASP B 208 <NA> -7.121 24.077 25.506  
## 3262 ATOM 3263 CB <NA> ASP B 208 <NA> -6.184 21.640 27.562  
## 3263 ATOM 3264 CG <NA> ASP B 208 <NA> -5.650 21.568 28.996  
## 3264 ATOM 3265 OD1 <NA> ASP B 208 <NA> -5.756 22.568 29.745  
## 3265 ATOM 3266 OD2 <NA> ASP B 208 <NA> -5.115 20.500 29.375  
## 3266 ATOM 3267 N <NA> LEU B 209 <NA> -8.170 22.138 25.149  
## 3267 ATOM 3268 CA <NA> LEU B 209 <NA> -8.394 22.423 23.740  
## 3268 ATOM 3269 C <NA> LEU B 209 <NA> -9.302 23.609 23.507  
## 3269 ATOM 3270 O <NA> LEU B 209 <NA> -9.132 24.335 22.538  
## 3270 ATOM 3271 CB <NA> LEU B 209 <NA> -9.020 21.241 23.072  
## 3271 ATOM 3272 CG <NA> LEU B 209 <NA> -8.174 20.026 23.285  
## 3272 ATOM 3273 CD1 <NA> LEU B 209 <NA> -8.897 18.846 22.676  
## 3273 ATOM 3274 CD2 <NA> LEU B 209 <NA> -6.801 20.287 22.664  
## 3274 ATOM 3275 N <NA> GLU B 210 <NA> -10.314 23.775 24.346  
## 3275 ATOM 3276 CA <NA> GLU B 210 <NA> -11.212 24.898 24.162  
## 3276 ATOM 3277 C <NA> GLU B 210 <NA> -10.431 26.168 24.374  
## 3277 ATOM 3278 O <NA> GLU B 210 <NA> -10.640 27.146 23.686  
## 3278 ATOM 3279 CB <NA> GLU B 210 <NA> -12.406 24.842 25.114  
## 3279 ATOM 3280 CG <NA> GLU B 210 <NA> -13.318 23.650 24.884  
## 3280 ATOM 3281 CD <NA> GLU B 210 <NA> -14.654 23.740 25.628  
## 3281 ATOM 3282 OE1 <NA> GLU B 210 <NA> -15.614 24.321 25.068  
## 3282 ATOM 3283 OE2 <NA> GLU B 210 <NA> -14.753 23.201 26.755  
## 3283 ATOM 3284 N <NA> LYS B 211 <NA> -9.507 26.148 25.320  
## 3284 ATOM 3285 CA <NA> LYS B 211 <NA> -8.704 27.330 25.596  
## 3285 ATOM 3286 C <NA> LYS B 211 <NA> -7.735 27.619 24.434  
## 3286 ATOM 3287 O <NA> LYS B 211 <NA> -7.508 28.777 24.055  
## 3287 ATOM 3288 CB <NA> LYS B 211 <NA> -7.903 27.134 26.887  
## 3288 ATOM 3289 CG <NA> LYS B 211 <NA> -8.714 26.980 28.181  
## 3289 ATOM 3290 CD <NA> LYS B 211 <NA> -7.919 26.162 29.235  
## 3290 ATOM 3291 CE <NA> LYS B 211 <NA> -6.450 26.626 29.374  
## 3291 ATOM 3292 NZ <NA> LYS B 211 <NA> -5.569 25.665 30.115  
## 3292 ATOM 3293 N <NA> ILE B 212 <NA> -7.191 26.553 23.860  
## 3293 ATOM 3294 CA <NA> ILE B 212 <NA> -6.231 26.655 22.765  
## 3294 ATOM 3295 C <NA> ILE B 212 <NA> -6.846 27.090 21.433  
## 3295 ATOM 3296 O <NA> ILE B 212 <NA> -6.295 27.937 20.741  
## 3296 ATOM 3297 CB <NA> ILE B 212 <NA> -5.489 25.293 22.576  
## 3297 ATOM 3298 CG1 <NA> ILE B 212 <NA> -4.590 25.005 23.784  
## 3298 ATOM 3299 CG2 <NA> ILE B 212 <NA> -4.688 25.286 21.278  
## 3299 ATOM 3300 CD1 <NA> ILE B 212 <NA> -4.251 23.537 23.963  
## 3300 ATOM 3301 N <NA> LEU B 213 <NA> -8.014 26.546 21.118  
## 3301 ATOM 3302 CA <NA> LEU B 213 <NA> -8.685 26.803 19.857  
## 3302 ATOM 3303 C <NA> LEU B 213 <NA> -9.702 27.928 19.804  
## 3303 ATOM 3304 O <NA> LEU B 213 <NA> -10.063 28.398 18.720  
## 3304 ATOM 3305 CB <NA> LEU B 213 <NA> -9.360 25.519 19.409  
## 3305 ATOM 3306 CG <NA> LEU B 213 <NA> -8.409 24.350 19.241  
## 3306 ATOM 3307 CD1 <NA> LEU B 213 <NA> -9.164 23.109 18.910  
## 3307 ATOM 3308 CD2 <NA> LEU B 213 <NA> -7.479 24.669 18.154  
## 3308 ATOM 3309 N <NA> GLY B 214 <NA> -10.182 28.343 20.963  
## 3309 ATOM 3310 CA <NA> GLY B 214 <NA> -11.180 29.388 21.013  
## 3310 ATOM 3311 C <NA> GLY B 214 <NA> -12.496 28.783 21.466  
## 3311 ATOM 3312 O <NA> GLY B 214 <NA> -13.318 29.510 22.074  
## 3312 ATOM 3313 OXT <NA> GLY B 214 <NA> -12.702 27.567 21.239  
## 3313 HETATM 3315 O <NA> HOH A 215 <NA> -0.994 -7.251 -18.028  
## 3314 HETATM 3316 O <NA> HOH A 216 <NA> 5.354 -12.406 -17.253  
## 3315 HETATM 3317 O <NA> HOH A 217 <NA> -14.469 -11.582 -8.421  
## 3316 HETATM 3318 O <NA> HOH A 218 <NA> -5.506 -7.345 -14.356  
## 3317 HETATM 3319 O <NA> HOH A 219 <NA> -20.909 -24.629 -8.331  
## 3318 HETATM 3320 O <NA> HOH A 220 <NA> 1.902 -10.139 -13.257  
## 3319 HETATM 3321 O <NA> HOH A 221 <NA> 3.410 -10.602 -10.980  
## 3320 HETATM 3322 O <NA> HOH A 222 <NA> 1.244 -25.981 -1.284  
## 3321 HETATM 3323 O <NA> HOH A 223 <NA> -5.799 -18.925 -36.379  
## 3322 HETATM 3324 O <NA> HOH A 224 <NA> 4.157 -9.983 -20.341  
## 3323 HETATM 3325 O <NA> HOH A 225 <NA> -6.976 -11.505 -24.948  
## 3324 HETATM 3326 O <NA> HOH A 226 <NA> 2.875 -20.840 -5.298  
## 3325 HETATM 3327 O <NA> HOH A 227 <NA> 11.626 -12.724 -7.430  
## 3326 HETATM 3328 O <NA> HOH A 228 <NA> 4.240 -22.792 -22.485  
## 3327 HETATM 3329 O <NA> HOH A 229 <NA> 6.681 3.656 -30.454  
## 3328 HETATM 3330 O <NA> HOH A 230 <NA> -8.324 -11.223 3.502  
## 3329 HETATM 3331 O <NA> HOH A 231 <NA> -19.208 -22.272 -3.129  
## 3330 HETATM 3332 O <NA> HOH A 232 <NA> -19.772 -21.325 -18.604  
## 3331 HETATM 3333 O <NA> HOH A 233 <NA> -3.167 -8.101 -25.662  
## 3332 HETATM 3334 O <NA> HOH A 234 <NA> 6.690 -2.659 -12.397  
## 3333 HETATM 3335 O <NA> HOH A 235 <NA> 9.500 -8.384 -25.238  
## 3334 HETATM 3336 O <NA> HOH A 236 <NA> -17.722 -13.002 -19.933  
## 3335 HETATM 3337 O <NA> HOH A 237 <NA> 18.567 -4.451 -8.407  
## 3336 HETATM 3338 O <NA> HOH A 238 <NA> 13.294 0.261 -29.130  
## 3337 HETATM 3339 O <NA> HOH A 239 <NA> 1.212 0.626 -18.070  
## 3338 HETATM 3340 O <NA> HOH A 240 <NA> -6.512 -21.331 2.984  
## 3339 HETATM 3341 O <NA> HOH A 241 <NA> -14.008 -20.822 -28.580  
## 3340 HETATM 3342 O <NA> HOH A 242 <NA> 7.966 -8.789 3.160  
## 3341 HETATM 3343 O <NA> HOH A 243 <NA> 1.525 -22.673 -4.335  
## 3342 HETATM 3344 O <NA> HOH A 244 <NA> 4.196 -16.329 -26.054  
## 3343 HETATM 3345 O <NA> HOH A 245 <NA> -5.986 -4.540 -24.096  
## 3344 HETATM 3346 O <NA> HOH A 246 <NA> -13.692 -4.958 -15.750  
## 3345 HETATM 3347 O <NA> HOH A 247 <NA> -8.339 -11.912 11.054  
## 3346 HETATM 3348 O <NA> HOH A 248 <NA> -16.182 -20.425 -6.267  
## 3347 HETATM 3349 O <NA> HOH A 249 <NA> 4.796 -22.464 -5.119  
## 3348 HETATM 3350 O <NA> HOH A 250 <NA> -5.259 -10.575 -27.096  
## 3349 HETATM 3351 O <NA> HOH A 251 <NA> -2.378 -4.013 -17.624  
## 3350 HETATM 3352 O <NA> HOH A 252 <NA> -11.215 -9.556 -5.190  
## 3351 HETATM 3353 O <NA> HOH A 253 <NA> 1.120 -25.877 -6.377  
## 3352 HETATM 3354 O <NA> HOH A 254 <NA> 3.670 -24.750 -6.983  
## 3353 HETATM 3355 O <NA> HOH A 255 <NA> 2.064 -15.589 6.718  
## 3354 HETATM 3356 O <NA> HOH A 256 <NA> 5.916 -7.322 -4.485  
## 3355 HETATM 3357 O <NA> HOH A 257 <NA> 0.683 -3.013 -30.059  
## 3356 HETATM 3358 O <NA> HOH A 258 <NA> -2.404 -8.369 -6.743  
## 3357 HETATM 3359 O <NA> HOH A 259 <NA> 8.938 -10.884 -1.562  
## 3358 HETATM 3360 O <NA> HOH A 260 <NA> 6.262 -10.042 -10.648  
## 3359 HETATM 3361 O <NA> HOH A 261 <NA> -6.681 -28.354 -6.680  
## 3360 HETATM 3362 O <NA> HOH A 262 <NA> 9.641 -11.553 -17.134  
## 3361 HETATM 3363 O <NA> HOH A 263 <NA> -14.246 -10.298 1.323  
## 3362 HETATM 3364 O <NA> HOH A 264 <NA> 0.107 -16.183 9.091  
## 3363 HETATM 3365 O <NA> HOH A 265 <NA> 5.921 -3.150 9.238  
## 3364 HETATM 3366 O <NA> HOH A 266 <NA> 3.507 9.531 -24.616  
## 3365 HETATM 3367 O <NA> HOH A 267 <NA> -10.454 -5.041 -24.718  
## 3366 HETATM 3368 O <NA> HOH A 268 <NA> 8.438 -30.492 -4.993  
## 3367 HETATM 3369 O <NA> HOH A 269 <NA> -17.004 -21.289 -26.195  
## 3368 HETATM 3370 O <NA> HOH A 270 <NA> 12.692 -4.165 -25.007  
## 3369 HETATM 3371 O <NA> HOH A 271 <NA> 7.307 -20.072 4.542  
## 3370 HETATM 3372 O <NA> HOH A 272 <NA> 4.134 8.717 -13.047  
## 3371 HETATM 3373 O <NA> HOH A 273 <NA> 6.316 -8.209 -22.135  
## 3372 HETATM 3374 O <NA> HOH A 274 <NA> 3.749 -35.579 -11.099  
## 3373 HETATM 3375 O <NA> HOH A 275 <NA> -12.660 -6.088 -2.099  
## 3374 HETATM 3376 O <NA> HOH A 276 <NA> -23.021 -12.987 -19.786  
## 3375 HETATM 3377 O <NA> HOH A 277 <NA> -7.812 -26.921 -31.097  
## 3376 HETATM 3378 O <NA> HOH A 278 <NA> -6.843 -27.882 -3.963  
## 3377 HETATM 3379 O <NA> HOH A 279 <NA> 14.841 -10.419 -8.955  
## 3378 HETATM 3380 O <NA> HOH A 280 <NA> -9.157 -7.749 -14.619  
## 3379 HETATM 3381 O <NA> HOH A 281 <NA> -4.737 -5.702 -17.778  
## 3380 HETATM 3382 O <NA> HOH A 282 <NA> -14.055 -21.945 0.062  
## 3381 HETATM 3383 O <NA> HOH A 283 <NA> 0.503 4.011 -18.475  
## 3382 HETATM 3384 O <NA> HOH A 284 <NA> -10.783 1.443 -31.495  
## 3383 HETATM 3385 O <NA> HOH A 285 <NA> -16.560 -25.447 -15.472  
## 3384 HETATM 3386 O <NA> HOH A 286 <NA> 13.909 12.731 -19.034  
## 3385 HETATM 3387 O <NA> HOH B 215 <NA> 0.753 11.463 14.020  
## 3386 HETATM 3388 O <NA> HOH B 216 <NA> 2.312 22.427 5.982  
## 3387 HETATM 3389 O <NA> HOH B 217 <NA> 2.885 17.485 27.282  
## 3388 HETATM 3390 O <NA> HOH B 218 <NA> 2.618 26.125 7.165  
## 3389 HETATM 3391 O <NA> HOH B 219 <NA> 2.325 24.266 23.665  
## 3390 HETATM 3392 O <NA> HOH B 220 <NA> 10.842 14.205 7.658  
## 3391 HETATM 3393 O <NA> HOH B 221 <NA> -15.965 12.859 9.643  
## 3392 HETATM 3394 O <NA> HOH B 222 <NA> 4.269 13.139 18.790  
## 3393 HETATM 3395 O <NA> HOH B 223 <NA> 3.360 28.210 -3.895  
## 3394 HETATM 3396 O <NA> HOH B 224 <NA> 2.398 11.413 21.172  
## 3395 HETATM 3397 O <NA> HOH B 225 <NA> -0.109 8.945 13.965  
## 3396 HETATM 3398 O <NA> HOH B 226 <NA> -1.584 6.477 3.979  
## 3397 HETATM 3399 O <NA> HOH B 227 <NA> -17.397 21.840 7.336  
## 3398 HETATM 3400 O <NA> HOH B 228 <NA> 9.917 25.563 9.269  
## 3399 HETATM 3401 O <NA> HOH B 229 <NA> -10.366 10.643 31.926  
## 3400 HETATM 3402 O <NA> HOH B 230 <NA> -14.734 9.720 13.372  
## 3401 HETATM 3403 O <NA> HOH B 231 <NA> -18.444 13.762 6.167  
## 3402 HETATM 3404 O <NA> HOH B 232 <NA> 8.127 11.957 2.636  
## 3403 HETATM 3405 O <NA> HOH B 233 <NA> -3.193 9.423 7.826  
## 3404 HETATM 3406 O <NA> HOH B 234 <NA> 6.060 20.534 -3.950  
## 3405 HETATM 3407 O <NA> HOH B 235 <NA> 1.444 8.841 11.563  
## 3406 HETATM 3408 O <NA> HOH B 236 <NA> 0.661 24.643 5.340  
## 3407 HETATM 3409 O <NA> HOH B 237 <NA> -1.422 32.161 12.634  
## 3408 HETATM 3410 O <NA> HOH B 238 <NA> -14.655 19.548 30.014  
## 3409 HETATM 3411 O <NA> HOH B 239 <NA> -1.094 18.794 -6.500  
## 3410 HETATM 3412 O <NA> HOH B 240 <NA> -4.839 8.876 26.282  
## 3411 HETATM 3413 O <NA> HOH B 241 <NA> 6.166 -4.007 -8.187  
## 3412 HETATM 3414 O <NA> HOH B 242 <NA> -13.187 10.971 -4.425  
## 3413 HETATM 3415 O <NA> HOH B 243 <NA> 12.167 5.279 30.617  
## 3414 HETATM 3416 O <NA> HOH B 244 <NA> -2.429 20.391 27.492  
## 3415 HETATM 3417 O <NA> HOH B 245 <NA> -19.060 -11.700 19.382  
## 3416 HETATM 3418 O <NA> HOH B 246 <NA> 4.068 -3.134 -12.123  
## 3417 HETATM 3419 O <NA> HOH B 247 <NA> 0.396 -7.823 25.917  
## 3418 HETATM 3420 O <NA> HOH B 248 <NA> 2.908 12.653 11.870  
## 3419 HETATM 3421 O <NA> HOH B 249 <NA> -6.729 8.785 16.022  
## 3420 HETATM 3422 O <NA> HOH B 250 <NA> -2.963 5.487 17.788  
## 3421 HETATM 3423 O <NA> HOH B 251 <NA> -8.937 30.099 16.322  
## 3422 HETATM 3424 O <NA> HOH B 252 <NA> -7.788 23.114 -3.303  
## 3423 HETATM 3425 O <NA> HOH B 253 <NA> -5.794 31.947 22.656  
## 3424 HETATM 3426 O <NA> HOH B 254 <NA> 1.721 1.568 19.785  
## 3425 HETATM 3427 O <NA> HOH B 255 <NA> 0.088 0.636 33.846  
## 3426 HETATM 3428 O <NA> HOH B 256 <NA> 14.137 11.008 10.414  
## 3427 HETATM 3429 O <NA> HOH B 257 <NA> -14.880 14.842 25.870  
## 3428 HETATM 3430 O <NA> HOH B 258 <NA> -11.865 10.748 4.095  
## 3429 HETATM 3431 O <NA> HOH B 259 <NA> 5.231 8.477 5.868  
## 3430 HETATM 3432 O <NA> HOH B 260 <NA> 13.544 -0.100 20.626  
## 3431 HETATM 3433 O <NA> HOH B 261 <NA> 2.104 19.854 -4.819  
## 3432 HETATM 3434 O <NA> HOH B 262 <NA> -8.845 -18.232 20.878  
## 3433 HETATM 3435 O <NA> HOH B 263 <NA> -13.459 0.357 -9.212  
## 3434 HETATM 3436 O <NA> HOH B 264 <NA> 7.133 1.252 -3.944  
## 3435 HETATM 3437 O <NA> HOH B 265 <NA> -11.446 25.901 5.307  
## 3436 HETATM 3438 O <NA> HOH B 266 <NA> -6.113 28.286 6.064  
## 3437 HETATM 3439 O <NA> HOH B 267 <NA> 6.157 3.191 14.123  
## 3438 HETATM 3440 O <NA> HOH B 268 <NA> 0.066 20.607 30.154  
## 3439 HETATM 3441 O <NA> HOH B 269 <NA> -15.259 29.479 10.829  
## 3440 HETATM 3442 O <NA> HOH B 270 <NA> 7.636 16.857 -1.730  
## 3441 HETATM 3443 O <NA> HOH B 271 <NA> -12.551 12.651 32.344  
## 3442 HETATM 3444 O <NA> HOH B 272 <NA> -7.898 6.315 19.969  
## 3443 HETATM 3445 O <NA> HOH B 273 <NA> -3.329 8.187 12.148  
## 3444 HETATM 3446 O <NA> HOH B 274 <NA> 1.907 1.187 -11.049  
## 3445 HETATM 3447 O <NA> HOH B 275 <NA> -14.282 16.101 -5.765  
## 3446 HETATM 3448 O <NA> HOH B 276 <NA> -9.236 31.694 22.033  
## 3447 HETATM 3449 O <NA> HOH B 277 <NA> -9.297 -9.613 38.855  
## 3448 HETATM 3450 O <NA> HOH B 278 <NA> 11.235 32.152 12.896  
## 3449 HETATM 3451 O <NA> HOH B 279 <NA> 17.160 5.051 16.461  
## 3450 HETATM 3452 O <NA> HOH B 280 <NA> 3.990 -5.955 -10.589  
## 3451 HETATM 3453 O <NA> HOH B 281 <NA> 5.311 11.964 21.256  
## 3452 HETATM 3454 O <NA> HOH B 282 <NA> -14.335 13.829 22.078  
## 3453 HETATM 3455 O <NA> HOH B 283 <NA> 2.298 31.749 15.792  
## 3454 HETATM 3456 O <NA> HOH B 284 <NA> 5.546 10.385 23.586  
## 3455 HETATM 3457 O <NA> HOH B 285 <NA> -12.845 28.308 11.296  
## 3456 HETATM 3458 O <NA> HOH B 286 <NA> 12.329 34.095 16.314  
## 3457 HETATM 3459 O <NA> HOH B 287 <NA> 8.485 19.881 -0.784  
## 3458 HETATM 3460 O <NA> HOH B 288 <NA> -0.660 0.094 16.265  
## 3459 HETATM 3461 O <NA> HOH B 289 <NA> 1.413 -6.322 -9.968  
## o b segid elesy charge  
## 1 1.0 41.45 <NA> N <NA>  
## 2 1.0 29.02 <NA> C <NA>  
## 3 1.0 27.93 <NA> C <NA>  
## 4 1.0 26.35 <NA> O <NA>  
## 5 1.0 34.19 <NA> C <NA>  
## 6 1.0 35.38 <NA> C <NA>  
## 7 1.0 47.23 <NA> S <NA>  
## 8 1.0 57.10 <NA> C <NA>  
## 9 1.0 18.86 <NA> N <NA>  
## 10 1.0 18.44 <NA> C <NA>  
## 11 1.0 17.92 <NA> C <NA>  
## 12 1.0 14.33 <NA> O <NA>  
## 13 1.0 15.82 <NA> C <NA>  
## 14 1.0 14.62 <NA> C <NA>  
## 15 1.0 16.76 <NA> C <NA>  
## 16 1.0 26.82 <NA> N <NA>  
## 17 1.0 22.35 <NA> C <NA>  
## 18 1.0 17.01 <NA> N <NA>  
## 19 1.0 21.25 <NA> N <NA>  
## 20 1.0 19.81 <NA> N <NA>  
## 21 1.0 16.20 <NA> C <NA>  
## 22 1.0 18.99 <NA> C <NA>  
## 23 1.0 20.46 <NA> O <NA>  
## 24 1.0 20.46 <NA> C <NA>  
## 25 1.0 18.10 <NA> C <NA>  
## 26 1.0 14.03 <NA> C <NA>  
## 27 1.0 14.32 <NA> C <NA>  
## 28 1.0 18.85 <NA> N <NA>  
## 29 1.0 19.67 <NA> C <NA>  
## 30 1.0 24.54 <NA> C <NA>  
## 31 1.0 19.52 <NA> O <NA>  
## 32 1.0 21.12 <NA> C <NA>  
## 33 1.0 20.62 <NA> C <NA>  
## 34 1.0 17.31 <NA> C <NA>  
## 35 1.0 19.71 <NA> C <NA>  
## 36 1.0 26.15 <NA> N <NA>  
## 37 1.0 20.26 <NA> C <NA>  
## 38 1.0 14.75 <NA> C <NA>  
## 39 1.0 15.92 <NA> O <NA>  
## 40 1.0 22.03 <NA> C <NA>  
## 41 1.0 28.96 <NA> C <NA>  
## 42 1.0 25.32 <NA> C <NA>  
## 43 1.0 28.87 <NA> C <NA>  
## 44 1.0 20.24 <NA> N <NA>  
## 45 1.0 20.55 <NA> C <NA>  
## 46 1.0 21.72 <NA> C <NA>  
## 47 1.0 23.55 <NA> O <NA>  
## 48 1.0 20.72 <NA> C <NA>  
## 49 1.0 14.85 <NA> C <NA>  
## 50 1.0 22.94 <NA> C <NA>  
## 51 1.0 10.35 <NA> C <NA>  
## 52 1.0 22.64 <NA> N <NA>  
## 53 1.0 17.05 <NA> C <NA>  
## 54 1.0 19.56 <NA> C <NA>  
## 55 1.0 25.37 <NA> O <NA>  
## 56 1.0 24.85 <NA> N <NA>  
## 57 1.0 22.13 <NA> C <NA>  
## 58 1.0 20.74 <NA> C <NA>  
## 59 1.0 23.78 <NA> O <NA>  
## 60 1.0 23.27 <NA> C <NA>  
## 61 1.0 24.92 <NA> N <NA>  
## 62 1.0 26.71 <NA> C <NA>  
## 63 1.0 27.23 <NA> C <NA>  
## 64 1.0 23.37 <NA> O <NA>  
## 65 1.0 24.88 <NA> C <NA>  
## 66 1.0 20.70 <NA> C <NA>  
## 67 1.0 14.95 <NA> C <NA>  
## 68 1.0 23.82 <NA> N <NA>  
## 69 1.0 33.05 <NA> C <NA>  
## 70 1.0 40.02 <NA> C <NA>  
## 71 1.0 49.11 <NA> O <NA>  
## 72 1.0 35.18 <NA> N <NA>  
## 73 1.0 30.66 <NA> C <NA>  
## 74 1.0 35.56 <NA> C <NA>  
## 75 1.0 44.64 <NA> O <NA>  
## 76 1.0 27.34 <NA> C <NA>  
## 77 1.0 38.51 <NA> N <NA>  
## 78 1.0 32.73 <NA> C <NA>  
## 79 1.0 35.11 <NA> C <NA>  
## 80 1.0 32.17 <NA> O <NA>  
## 81 1.0 28.70 <NA> N <NA>  
## 82 1.0 25.61 <NA> C <NA>  
## 83 1.0 20.57 <NA> C <NA>  
## 84 1.0 25.81 <NA> O <NA>  
## 85 1.0 24.52 <NA> C <NA>  
## 86 1.0 31.99 <NA> C <NA>  
## 87 1.0 28.69 <NA> C <NA>  
## 88 1.0 25.37 <NA> C <NA>  
## 89 1.0 37.66 <NA> N <NA>  
## 90 1.0 25.26 <NA> N <NA>  
## 91 1.0 33.19 <NA> C <NA>  
## 92 1.0 36.66 <NA> C <NA>  
## 93 1.0 47.14 <NA> O <NA>  
## 94 1.0 43.58 <NA> N <NA>  
## 95 1.0 41.03 <NA> C <NA>  
## 96 1.0 35.16 <NA> C <NA>  
## 97 1.0 41.12 <NA> O <NA>  
## 98 1.0 39.87 <NA> C <NA>  
## 99 1.0 33.22 <NA> O <NA>  
## 100 1.0 30.71 <NA> C <NA>  
## 101 1.0 27.06 <NA> N <NA>  
## 102 1.0 24.09 <NA> C <NA>  
## 103 1.0 15.76 <NA> C <NA>  
## 104 1.0 21.86 <NA> O <NA>  
## 105 1.0 32.98 <NA> C <NA>  
## 106 1.0 44.76 <NA> C <NA>  
## 107 1.0 45.91 <NA> C <NA>  
## 108 1.0 42.94 <NA> O <NA>  
## 109 1.0 53.87 <NA> N <NA>  
## 110 1.0 15.73 <NA> N <NA>  
## 111 1.0 16.18 <NA> C <NA>  
## 112 1.0 21.83 <NA> C <NA>  
## 113 1.0 30.75 <NA> O <NA>  
## 114 1.0 18.36 <NA> C <NA>  
## 115 1.0 24.00 <NA> N <NA>  
## 116 1.0 19.14 <NA> C <NA>  
## 117 1.0 23.02 <NA> C <NA>  
## 118 1.0 28.87 <NA> O <NA>  
## 119 1.0 30.86 <NA> C <NA>  
## 120 1.0 39.30 <NA> C <NA>  
## 121 1.0 46.90 <NA> C <NA>  
## 122 1.0 47.07 <NA> O <NA>  
## 123 1.0 49.60 <NA> N <NA>  
## 124 1.0 24.58 <NA> N <NA>  
## 125 1.0 29.19 <NA> C <NA>  
## 126 1.0 25.55 <NA> C <NA>  
## 127 1.0 30.03 <NA> O <NA>  
## 128 1.0 31.02 <NA> C <NA>  
## 129 1.0 37.88 <NA> C <NA>  
## 130 1.0 41.93 <NA> C <NA>  
## 131 1.0 37.56 <NA> C <NA>  
## 132 1.0 36.63 <NA> C <NA>  
## 133 1.0 36.09 <NA> C <NA>  
## 134 1.0 38.23 <NA> C <NA>  
## 135 1.0 21.71 <NA> N <NA>  
## 136 1.0 14.79 <NA> C <NA>  
## 137 1.0 15.12 <NA> C <NA>  
## 138 1.0 22.51 <NA> O <NA>  
## 139 1.0 19.28 <NA> C <NA>  
## 140 1.0 12.35 <NA> C <NA>  
## 141 1.0 22.13 <NA> C <NA>  
## 142 1.0 11.81 <NA> C <NA>  
## 143 1.0 20.31 <NA> N <NA>  
## 144 1.0 19.63 <NA> C <NA>  
## 145 1.0 25.58 <NA> C <NA>  
## 146 1.0 22.94 <NA> O <NA>  
## 147 1.0 14.43 <NA> C <NA>  
## 148 1.0 9.52 <NA> C <NA>  
## 149 1.0 25.46 <NA> S <NA>  
## 150 1.0 25.48 <NA> C <NA>  
## 151 1.0 29.08 <NA> N <NA>  
## 152 1.0 28.54 <NA> C <NA>  
## 153 1.0 30.09 <NA> C <NA>  
## 154 1.0 35.19 <NA> O <NA>  
## 155 1.0 33.18 <NA> C <NA>  
## 156 1.0 51.95 <NA> C <NA>  
## 157 1.0 62.16 <NA> C <NA>  
## 158 1.0 66.90 <NA> O <NA>  
## 159 1.0 69.38 <NA> O <NA>  
## 160 1.0 28.67 <NA> N <NA>  
## 161 1.0 27.49 <NA> C <NA>  
## 162 1.0 31.92 <NA> C <NA>  
## 163 1.0 35.62 <NA> O <NA>  
## 164 1.0 37.77 <NA> C <NA>  
## 165 1.0 52.92 <NA> C <NA>  
## 166 1.0 60.30 <NA> C <NA>  
## 167 1.0 67.95 <NA> C <NA>  
## 168 1.0 76.00 <NA> N <NA>  
## 169 1.0 33.47 <NA> N <NA>  
## 170 1.0 32.56 <NA> C <NA>  
## 171 1.0 29.46 <NA> C <NA>  
## 172 1.0 30.64 <NA> O <NA>  
## 173 1.0 39.55 <NA> C <NA>  
## 174 1.0 49.14 <NA> C <NA>  
## 175 1.0 54.90 <NA> C <NA>  
## 176 1.0 51.82 <NA> C <NA>  
## 177 1.0 58.34 <NA> C <NA>  
## 178 1.0 58.23 <NA> C <NA>  
## 179 1.0 61.65 <NA> C <NA>  
## 180 1.0 59.62 <NA> O <NA>  
## 181 1.0 15.62 <NA> N <NA>  
## 182 1.0 17.13 <NA> C <NA>  
## 183 1.0 18.90 <NA> C <NA>  
## 184 1.0 28.06 <NA> O <NA>  
## 185 1.0 23.56 <NA> N <NA>  
## 186 1.0 15.50 <NA> C <NA>  
## 187 1.0 11.25 <NA> C <NA>  
## 188 1.0 18.41 <NA> O <NA>  
## 189 1.0 12.49 <NA> C <NA>  
## 190 1.0 13.87 <NA> C <NA>  
## 191 1.0 16.25 <NA> C <NA>  
## 192 1.0 10.29 <NA> C <NA>  
## 193 1.0 14.01 <NA> N <NA>  
## 194 1.0 6.98 <NA> C <NA>  
## 195 1.0 13.79 <NA> C <NA>  
## 196 1.0 17.64 <NA> O <NA>  
## 197 1.0 13.98 <NA> C <NA>  
## 198 1.0 9.57 <NA> C <NA>  
## 199 1.0 15.19 <NA> C <NA>  
## 200 1.0 20.42 <NA> N <NA>  
## 201 1.0 24.07 <NA> C <NA>  
## 202 1.0 26.26 <NA> C <NA>  
## 203 1.0 29.64 <NA> O <NA>  
## 204 1.0 24.47 <NA> C <NA>  
## 205 1.0 26.13 <NA> C <NA>  
## 206 1.0 34.52 <NA> C <NA>  
## 207 1.0 34.10 <NA> O <NA>  
## 208 1.0 41.73 <NA> N <NA>  
## 209 1.0 32.32 <NA> N <NA>  
## 210 1.0 24.00 <NA> C <NA>  
## 211 1.0 21.87 <NA> C <NA>  
## 212 1.0 24.59 <NA> O <NA>  
## 213 1.0 27.73 <NA> C <NA>  
## 214 1.0 15.14 <NA> C <NA>  
## 215 1.0 31.71 <NA> C <NA>  
## 216 1.0 17.03 <NA> C <NA>  
## 217 1.0 25.51 <NA> N <NA>  
## 218 1.0 23.94 <NA> C <NA>  
## 219 1.0 29.33 <NA> C <NA>  
## 220 1.0 34.68 <NA> O <NA>  
## 221 1.0 16.98 <NA> C <NA>  
## 222 1.0 38.68 <NA> O <NA>  
## 223 1.0 34.57 <NA> N <NA>  
## 224 1.0 30.70 <NA> C <NA>  
## 225 1.0 28.86 <NA> C <NA>  
## 226 1.0 32.98 <NA> O <NA>  
## 227 1.0 31.15 <NA> C <NA>  
## 228 1.0 24.39 <NA> O <NA>  
## 229 1.0 22.57 <NA> C <NA>  
## 230 1.0 30.48 <NA> N <NA>  
## 231 1.0 24.70 <NA> C <NA>  
## 232 1.0 29.25 <NA> C <NA>  
## 233 1.0 39.43 <NA> O <NA>  
## 234 1.0 32.74 <NA> N <NA>  
## 235 1.0 32.84 <NA> C <NA>  
## 236 1.0 30.19 <NA> C <NA>  
## 237 1.0 34.33 <NA> O <NA>  
## 238 1.0 46.88 <NA> C <NA>  
## 239 1.0 60.27 <NA> C <NA>  
## 240 1.0 62.94 <NA> O <NA>  
## 241 1.0 71.64 <NA> O <NA>  
## 242 1.0 37.94 <NA> N <NA>  
## 243 1.0 34.60 <NA> C <NA>  
## 244 1.0 34.65 <NA> C <NA>  
## 245 1.0 37.79 <NA> O <NA>  
## 246 1.0 30.39 <NA> C <NA>  
## 247 1.0 38.60 <NA> C <NA>  
## 248 1.0 43.86 <NA> S <NA>  
## 249 1.0 53.38 <NA> C <NA>  
## 250 1.0 32.63 <NA> N <NA>  
## 251 1.0 33.01 <NA> C <NA>  
## 252 1.0 37.17 <NA> C <NA>  
## 253 1.0 44.58 <NA> O <NA>  
## 254 1.0 37.24 <NA> C <NA>  
## 255 1.0 43.99 <NA> C <NA>  
## 256 1.0 45.97 <NA> C <NA>  
## 257 1.0 43.67 <NA> C <NA>  
## 258 1.0 40.18 <NA> N <NA>  
## 259 1.0 44.60 <NA> C <NA>  
## 260 1.0 43.82 <NA> C <NA>  
## 261 1.0 50.27 <NA> O <NA>  
## 262 1.0 42.88 <NA> C <NA>  
## 263 1.0 44.29 <NA> C <NA>  
## 264 1.0 53.07 <NA> C <NA>  
## 265 1.0 60.98 <NA> N <NA>  
## 266 1.0 68.24 <NA> C <NA>  
## 267 1.0 72.51 <NA> N <NA>  
## 268 1.0 68.98 <NA> N <NA>  
## 269 1.0 46.52 <NA> N <NA>  
## 270 1.0 50.74 <NA> C <NA>  
## 271 1.0 58.10 <NA> C <NA>  
## 272 1.0 57.67 <NA> O <NA>  
## 273 1.0 56.71 <NA> C <NA>  
## 274 1.0 61.85 <NA> N <NA>  
## 275 1.0 57.32 <NA> C <NA>  
## 276 1.0 53.79 <NA> C <NA>  
## 277 1.0 52.54 <NA> O <NA>  
## 278 1.0 59.46 <NA> C <NA>  
## 279 1.0 47.91 <NA> N <NA>  
## 280 1.0 47.04 <NA> C <NA>  
## 281 1.0 52.43 <NA> C <NA>  
## 282 1.0 55.56 <NA> O <NA>  
## 283 1.0 41.46 <NA> C <NA>  
## 284 1.0 47.42 <NA> C <NA>  
## 285 1.0 42.93 <NA> C <NA>  
## 286 1.0 59.78 <NA> N <NA>  
## 287 1.0 67.13 <NA> C <NA>  
## 288 1.0 71.55 <NA> C <NA>  
## 289 1.0 77.25 <NA> O <NA>  
## 290 1.0 66.92 <NA> C <NA>  
## 291 1.0 65.44 <NA> C <NA>  
## 292 1.0 71.73 <NA> C <NA>  
## 293 1.0 67.86 <NA> C <NA>  
## 294 1.0 64.01 <NA> N <NA>  
## 295 1.0 74.97 <NA> N <NA>  
## 296 1.0 81.04 <NA> C <NA>  
## 297 1.0 83.60 <NA> C <NA>  
## 298 1.0 88.86 <NA> O <NA>  
## 299 1.0 84.97 <NA> C <NA>  
## 300 1.0 98.23 <NA> O <NA>  
## 301 1.0 81.63 <NA> N <NA>  
## 302 1.0 75.20 <NA> C <NA>  
## 303 1.0 69.46 <NA> C <NA>  
## 304 1.0 72.12 <NA> O <NA>  
## 305 1.0 64.93 <NA> N <NA>  
## 306 1.0 59.68 <NA> C <NA>  
## 307 1.0 56.65 <NA> C <NA>  
## 308 1.0 51.43 <NA> O <NA>  
## 309 1.0 61.71 <NA> C <NA>  
## 310 1.0 62.31 <NA> O <NA>  
## 311 1.0 55.07 <NA> N <NA>  
## 312 1.0 55.63 <NA> C <NA>  
## 313 1.0 53.88 <NA> C <NA>  
## 314 1.0 53.83 <NA> O <NA>  
## 315 1.0 63.89 <NA> C <NA>  
## 316 1.0 78.12 <NA> C <NA>  
## 317 1.0 83.24 <NA> C <NA>  
## 318 1.0 86.87 <NA> O <NA>  
## 319 1.0 83.37 <NA> O <NA>  
## 320 1.0 49.26 <NA> N <NA>  
## 321 1.0 45.12 <NA> C <NA>  
## 322 1.0 48.23 <NA> C <NA>  
## 323 1.0 44.66 <NA> O <NA>  
## 324 1.0 45.72 <NA> C <NA>  
## 325 1.0 48.49 <NA> C <NA>  
## 326 1.0 53.63 <NA> C <NA>  
## 327 1.0 58.47 <NA> C <NA>  
## 328 1.0 47.60 <NA> N <NA>  
## 329 1.0 39.04 <NA> C <NA>  
## 330 1.0 35.03 <NA> C <NA>  
## 331 1.0 34.68 <NA> O <NA>  
## 332 1.0 39.91 <NA> N <NA>  
## 333 1.0 44.31 <NA> C <NA>  
## 334 1.0 44.85 <NA> C <NA>  
## 335 1.0 48.38 <NA> O <NA>  
## 336 1.0 56.95 <NA> C <NA>  
## 337 1.0 64.66 <NA> C <NA>  
## 338 1.0 69.88 <NA> C <NA>  
## 339 1.0 72.38 <NA> C <NA>  
## 340 1.0 73.54 <NA> N <NA>  
## 341 1.0 41.88 <NA> N <NA>  
## 342 1.0 38.21 <NA> C <NA>  
## 343 1.0 37.63 <NA> C <NA>  
## 344 1.0 46.52 <NA> O <NA>  
## 345 1.0 34.16 <NA> C <NA>  
## 346 1.0 34.59 <NA> C <NA>  
## 347 1.0 40.52 <NA> C <NA>  
## 348 1.0 45.57 <NA> O <NA>  
## 349 1.0 43.01 <NA> N <NA>  
## 350 1.0 39.47 <NA> N <NA>  
## 351 1.0 43.70 <NA> C <NA>  
## 352 1.0 43.34 <NA> C <NA>  
## 353 1.0 39.64 <NA> O <NA>  
## 354 1.0 48.96 <NA> C <NA>  
## 355 1.0 45.45 <NA> N <NA>  
## 356 1.0 44.19 <NA> C <NA>  
## 357 1.0 43.72 <NA> C <NA>  
## 358 1.0 43.88 <NA> O <NA>  
## 359 1.0 40.76 <NA> C <NA>  
## 360 1.0 43.34 <NA> C <NA>  
## 361 1.0 55.19 <NA> C <NA>  
## 362 1.0 60.91 <NA> C <NA>  
## 363 1.0 66.33 <NA> N <NA>  
## 364 1.0 44.35 <NA> N <NA>  
## 365 1.0 47.00 <NA> C <NA>  
## 366 1.0 45.24 <NA> C <NA>  
## 367 1.0 52.31 <NA> O <NA>  
## 368 1.0 57.14 <NA> C <NA>  
## 369 1.0 58.36 <NA> C <NA>  
## 370 1.0 58.71 <NA> O <NA>  
## 371 1.0 61.95 <NA> O <NA>  
## 372 1.0 49.01 <NA> N <NA>  
## 373 1.0 48.67 <NA> C <NA>  
## 374 1.0 41.70 <NA> C <NA>  
## 375 1.0 41.14 <NA> O <NA>  
## 376 1.0 52.20 <NA> C <NA>  
## 377 1.0 44.00 <NA> C <NA>  
## 378 1.0 51.87 <NA> C <NA>  
## 379 1.0 46.08 <NA> C <NA>  
## 380 1.0 42.06 <NA> N <NA>  
## 381 1.0 41.54 <NA> C <NA>  
## 382 1.0 42.02 <NA> C <NA>  
## 383 1.0 43.31 <NA> O <NA>  
## 384 1.0 47.40 <NA> C <NA>  
## 385 1.0 56.02 <NA> C <NA>  
## 386 1.0 77.33 <NA> S <NA>  
## 387 1.0 59.25 <NA> C <NA>  
## 388 1.0 46.64 <NA> N <NA>  
## 389 1.0 50.22 <NA> C <NA>  
## 390 1.0 50.20 <NA> C <NA>  
## 391 1.0 58.95 <NA> O <NA>  
## 392 1.0 48.85 <NA> C <NA>  
## 393 1.0 47.43 <NA> C <NA>  
## 394 1.0 46.99 <NA> O <NA>  
## 395 1.0 44.24 <NA> O <NA>  
## 396 1.0 48.71 <NA> N <NA>  
## 397 1.0 45.07 <NA> C <NA>  
## 398 1.0 45.60 <NA> C <NA>  
## 399 1.0 46.75 <NA> O <NA>  
## 400 1.0 46.96 <NA> C <NA>  
## 401 1.0 49.46 <NA> N <NA>  
## 402 1.0 49.77 <NA> C <NA>  
## 403 1.0 51.82 <NA> C <NA>  
## 404 1.0 56.12 <NA> O <NA>  
## 405 1.0 55.57 <NA> N <NA>  
## 406 1.0 52.04 <NA> C <NA>  
## 407 1.0 53.24 <NA> C <NA>  
## 408 1.0 55.96 <NA> O <NA>  
## 409 1.0 53.89 <NA> C <NA>  
## 410 1.0 56.37 <NA> C <NA>  
## 411 1.0 67.15 <NA> C <NA>  
## 412 1.0 72.82 <NA> C <NA>  
## 413 1.0 74.93 <NA> N <NA>  
## 414 1.0 50.05 <NA> N <NA>  
## 415 1.0 44.82 <NA> C <NA>  
## 416 1.0 38.82 <NA> C <NA>  
## 417 1.0 36.31 <NA> O <NA>  
## 418 1.0 46.73 <NA> C <NA>  
## 419 1.0 46.84 <NA> C <NA>  
## 420 1.0 46.82 <NA> C <NA>  
## 421 1.0 43.59 <NA> C <NA>  
## 422 1.0 37.98 <NA> N <NA>  
## 423 1.0 39.75 <NA> C <NA>  
## 424 1.0 39.94 <NA> C <NA>  
## 425 1.0 42.76 <NA> O <NA>  
## 426 1.0 42.82 <NA> C <NA>  
## 427 1.0 36.80 <NA> C <NA>  
## 428 1.0 41.69 <NA> C <NA>  
## 429 1.0 36.76 <NA> N <NA>  
## 430 1.0 35.79 <NA> C <NA>  
## 431 1.0 35.29 <NA> C <NA>  
## 432 1.0 33.49 <NA> O <NA>  
## 433 1.0 38.89 <NA> C <NA>  
## 434 1.0 45.98 <NA> O <NA>  
## 435 1.0 42.18 <NA> C <NA>  
## 436 1.0 34.73 <NA> N <NA>  
## 437 1.0 38.92 <NA> C <NA>  
## 438 1.0 35.48 <NA> C <NA>  
## 439 1.0 37.40 <NA> O <NA>  
## 440 1.0 38.14 <NA> C <NA>  
## 441 1.0 32.51 <NA> C <NA>  
## 442 1.0 39.71 <NA> O <NA>  
## 443 1.0 32.57 <NA> O <NA>  
## 444 1.0 35.37 <NA> N <NA>  
## 445 1.0 37.93 <NA> C <NA>  
## 446 1.0 30.79 <NA> C <NA>  
## 447 1.0 30.98 <NA> O <NA>  
## 448 1.0 50.69 <NA> C <NA>  
## 449 1.0 69.90 <NA> C <NA>  
## 450 1.0 71.20 <NA> C <NA>  
## 451 1.0 78.26 <NA> O <NA>  
## 452 1.0 73.01 <NA> O <NA>  
## 453 1.0 29.97 <NA> N <NA>  
## 454 1.0 27.18 <NA> C <NA>  
## 455 1.0 26.99 <NA> C <NA>  
## 456 1.0 31.63 <NA> O <NA>  
## 457 1.0 31.57 <NA> C <NA>  
## 458 1.0 32.06 <NA> C <NA>  
## 459 1.0 39.25 <NA> C <NA>  
## 460 1.0 38.77 <NA> C <NA>  
## 461 1.0 25.11 <NA> N <NA>  
## 462 1.0 26.86 <NA> C <NA>  
## 463 1.0 23.54 <NA> C <NA>  
## 464 1.0 36.24 <NA> O <NA>  
## 465 1.0 29.01 <NA> C <NA>  
## 466 1.0 22.83 <NA> C <NA>  
## 467 1.0 35.77 <NA> C <NA>  
## 468 1.0 32.40 <NA> N <NA>  
## 469 1.0 27.53 <NA> C <NA>  
## 470 1.0 29.39 <NA> C <NA>  
## 471 1.0 32.27 <NA> O <NA>  
## 472 1.0 31.29 <NA> C <NA>  
## 473 1.0 29.25 <NA> C <NA>  
## 474 1.0 35.74 <NA> C <NA>  
## 475 1.0 29.01 <NA> C <NA>  
## 476 1.0 34.26 <NA> N <NA>  
## 477 1.0 31.16 <NA> C <NA>  
## 478 1.0 34.96 <NA> C <NA>  
## 479 1.0 36.19 <NA> O <NA>  
## 480 1.0 32.44 <NA> C <NA>  
## 481 1.0 32.65 <NA> N <NA>  
## 482 1.0 27.08 <NA> C <NA>  
## 483 1.0 23.61 <NA> C <NA>  
## 484 1.0 28.81 <NA> O <NA>  
## 485 1.0 35.03 <NA> C <NA>  
## 486 1.0 34.91 <NA> C <NA>  
## 487 1.0 31.64 <NA> C <NA>  
## 488 1.0 34.52 <NA> C <NA>  
## 489 1.0 23.77 <NA> N <NA>  
## 490 1.0 23.03 <NA> C <NA>  
## 491 1.0 25.05 <NA> C <NA>  
## 492 1.0 36.11 <NA> O <NA>  
## 493 1.0 21.51 <NA> C <NA>  
## 494 1.0 22.42 <NA> C <NA>  
## 495 1.0 12.79 <NA> C <NA>  
## 496 1.0 28.92 <NA> N <NA>  
## 497 1.0 28.12 <NA> C <NA>  
## 498 1.0 28.95 <NA> C <NA>  
## 499 1.0 28.87 <NA> O <NA>  
## 500 1.0 30.34 <NA> C <NA>  
## 501 1.0 33.34 <NA> C <NA>  
## 502 1.0 57.12 <NA> C <NA>  
## 503 1.0 68.29 <NA> C <NA>  
## 504 1.0 73.65 <NA> N <NA>  
## 505 1.0 18.82 <NA> N <NA>  
## 506 1.0 24.78 <NA> C <NA>  
## 507 1.0 34.43 <NA> C <NA>  
## 508 1.0 40.57 <NA> O <NA>  
## 509 1.0 30.48 <NA> C <NA>  
## 510 1.0 47.35 <NA> C <NA>  
## 511 1.0 53.03 <NA> C <NA>  
## 512 1.0 64.48 <NA> O <NA>  
## 513 1.0 57.87 <NA> O <NA>  
## 514 1.0 33.55 <NA> N <NA>  
## 515 1.0 24.22 <NA> C <NA>  
## 516 1.0 23.57 <NA> C <NA>  
## 517 1.0 29.81 <NA> O <NA>  
## 518 1.0 26.48 <NA> C <NA>  
## 519 1.0 21.89 <NA> C <NA>  
## 520 1.0 27.49 <NA> C <NA>  
## 521 1.0 28.17 <NA> N <NA>  
## 522 1.0 30.25 <NA> C <NA>  
## 523 1.0 32.98 <NA> N <NA>  
## 524 1.0 38.84 <NA> N <NA>  
## 525 1.0 21.61 <NA> N <NA>  
## 526 1.0 18.69 <NA> C <NA>  
## 527 1.0 24.84 <NA> C <NA>  
## 528 1.0 28.83 <NA> O <NA>  
## 529 1.0 21.29 <NA> C <NA>  
## 530 1.0 19.14 <NA> C <NA>  
## 531 1.0 15.87 <NA> C <NA>  
## 532 1.0 30.14 <NA> C <NA>  
## 533 1.0 34.95 <NA> N <NA>  
## 534 1.0 40.67 <NA> C <NA>  
## 535 1.0 45.62 <NA> C <NA>  
## 536 1.0 47.72 <NA> O <NA>  
## 537 1.0 35.58 <NA> C <NA>  
## 538 1.0 42.96 <NA> N <NA>  
## 539 1.0 38.08 <NA> C <NA>  
## 540 1.0 41.23 <NA> C <NA>  
## 541 1.0 39.18 <NA> O <NA>  
## 542 1.0 29.08 <NA> C <NA>  
## 543 1.0 39.76 <NA> C <NA>  
## 544 1.0 57.07 <NA> C <NA>  
## 545 1.0 60.07 <NA> O <NA>  
## 546 1.0 64.32 <NA> N <NA>  
## 547 1.0 48.96 <NA> N <NA>  
## 548 1.0 55.26 <NA> C <NA>  
## 549 1.0 51.88 <NA> C <NA>  
## 550 1.0 48.34 <NA> O <NA>  
## 551 1.0 69.32 <NA> C <NA>  
## 552 1.0 79.10 <NA> C <NA>  
## 553 1.0 84.19 <NA> C <NA>  
## 554 1.0 88.37 <NA> O <NA>  
## 555 1.0 84.11 <NA> O <NA>  
## 556 1.0 49.64 <NA> N <NA>  
## 557 1.0 46.29 <NA> C <NA>  
## 558 1.0 44.15 <NA> C <NA>  
## 559 1.0 40.68 <NA> O <NA>  
## 560 1.0 36.81 <NA> C <NA>  
## 561 1.0 31.41 <NA> C <NA>  
## 562 1.0 32.06 <NA> O <NA>  
## 563 1.0 32.87 <NA> O <NA>  
## 564 1.0 34.50 <NA> N <NA>  
## 565 1.0 26.25 <NA> C <NA>  
## 566 1.0 22.86 <NA> C <NA>  
## 567 1.0 30.27 <NA> O <NA>  
## 568 1.0 9.52 <NA> C <NA>  
## 569 1.0 26.99 <NA> S <NA>  
## 570 1.0 32.83 <NA> N <NA>  
## 571 1.0 37.14 <NA> C <NA>  
## 572 1.0 37.85 <NA> C <NA>  
## 573 1.0 43.84 <NA> O <NA>  
## 574 1.0 47.41 <NA> C <NA>  
## 575 1.0 62.01 <NA> C <NA>  
## 576 1.0 73.31 <NA> C <NA>  
## 577 1.0 82.29 <NA> N <NA>  
## 578 1.0 85.11 <NA> C <NA>  
## 579 1.0 83.75 <NA> N <NA>  
## 580 1.0 81.84 <NA> N <NA>  
## 581 1.0 34.73 <NA> N <NA>  
## 582 1.0 27.50 <NA> C <NA>  
## 583 1.0 22.09 <NA> C <NA>  
## 584 1.0 25.67 <NA> O <NA>  
## 585 1.0 34.13 <NA> C <NA>  
## 586 1.0 36.90 <NA> C <NA>  
## 587 1.0 36.68 <NA> O <NA>  
## 588 1.0 45.32 <NA> N <NA>  
## 589 1.0 17.69 <NA> N <NA>  
## 590 1.0 16.86 <NA> C <NA>  
## 591 1.0 17.27 <NA> C <NA>  
## 592 1.0 15.83 <NA> O <NA>  
## 593 1.0 20.66 <NA> N <NA>  
## 594 1.0 27.76 <NA> C <NA>  
## 595 1.0 26.50 <NA> C <NA>  
## 596 1.0 28.02 <NA> O <NA>  
## 597 1.0 29.10 <NA> C <NA>  
## 598 1.0 33.16 <NA> C <NA>  
## 599 1.0 31.40 <NA> C <NA>  
## 600 1.0 27.09 <NA> C <NA>  
## 601 1.0 32.43 <NA> C <NA>  
## 602 1.0 32.66 <NA> C <NA>  
## 603 1.0 30.97 <NA> C <NA>  
## 604 1.0 22.30 <NA> N <NA>  
## 605 1.0 19.27 <NA> C <NA>  
## 606 1.0 19.29 <NA> C <NA>  
## 607 1.0 20.16 <NA> O <NA>  
## 608 1.0 19.17 <NA> C <NA>  
## 609 1.0 20.14 <NA> C <NA>  
## 610 1.0 12.74 <NA> C <NA>  
## 611 1.0 16.91 <NA> C <NA>  
## 612 1.0 22.96 <NA> N <NA>  
## 613 1.0 22.22 <NA> C <NA>  
## 614 1.0 20.44 <NA> C <NA>  
## 615 1.0 17.82 <NA> O <NA>  
## 616 1.0 23.11 <NA> C <NA>  
## 617 1.0 27.73 <NA> C <NA>  
## 618 1.0 37.32 <NA> C <NA>  
## 619 1.0 30.13 <NA> C <NA>  
## 620 1.0 22.61 <NA> N <NA>  
## 621 1.0 26.70 <NA> C <NA>  
## 622 1.0 29.03 <NA> C <NA>  
## 623 1.0 26.81 <NA> O <NA>  
## 624 1.0 24.75 <NA> C <NA>  
## 625 1.0 29.12 <NA> C <NA>  
## 626 1.0 40.54 <NA> O <NA>  
## 627 1.0 38.89 <NA> O <NA>  
## 628 1.0 31.06 <NA> N <NA>  
## 629 1.0 25.52 <NA> C <NA>  
## 630 1.0 35.02 <NA> C <NA>  
## 631 1.0 40.79 <NA> O <NA>  
## 632 1.0 32.55 <NA> N <NA>  
## 633 1.0 21.22 <NA> C <NA>  
## 634 1.0 17.96 <NA> C <NA>  
## 635 1.0 19.83 <NA> O <NA>  
## 636 1.0 23.81 <NA> C <NA>  
## 637 1.0 29.66 <NA> C <NA>  
## 638 1.0 19.34 <NA> C <NA>  
## 639 1.0 29.71 <NA> C <NA>  
## 640 1.0 20.42 <NA> C <NA>  
## 641 1.0 16.47 <NA> C <NA>  
## 642 1.0 14.00 <NA> C <NA>  
## 643 1.0 17.36 <NA> N <NA>  
## 644 1.0 15.90 <NA> C <NA>  
## 645 1.0 17.32 <NA> C <NA>  
## 646 1.0 25.25 <NA> O <NA>  
## 647 1.0 12.44 <NA> C <NA>  
## 648 1.0 14.93 <NA> C <NA>  
## 649 1.0 14.28 <NA> C <NA>  
## 650 1.0 13.73 <NA> N <NA>  
## 651 1.0 15.84 <NA> C <NA>  
## 652 1.0 28.17 <NA> C <NA>  
## 653 1.0 28.27 <NA> O <NA>  
## 654 1.0 16.22 <NA> C <NA>  
## 655 1.0 22.11 <NA> C <NA>  
## 656 1.0 21.72 <NA> C <NA>  
## 657 1.0 48.47 <NA> N <NA>  
## 658 1.0 51.56 <NA> C <NA>  
## 659 1.0 48.80 <NA> N <NA>  
## 660 1.0 49.01 <NA> N <NA>  
## 661 1.0 27.78 <NA> N <NA>  
## 662 1.0 22.44 <NA> C <NA>  
## 663 1.0 23.02 <NA> C <NA>  
## 664 1.0 29.88 <NA> O <NA>  
## 665 1.0 20.50 <NA> C <NA>  
## 666 1.0 26.51 <NA> O <NA>  
## 667 1.0 19.20 <NA> C <NA>  
## 668 1.0 27.74 <NA> N <NA>  
## 669 1.0 19.61 <NA> C <NA>  
## 670 1.0 18.78 <NA> C <NA>  
## 671 1.0 23.93 <NA> O <NA>  
## 672 1.0 21.39 <NA> C <NA>  
## 673 1.0 21.41 <NA> C <NA>  
## 674 1.0 15.36 <NA> C <NA>  
## 675 1.0 22.52 <NA> C <NA>  
## 676 1.0 20.68 <NA> N <NA>  
## 677 1.0 21.23 <NA> C <NA>  
## 678 1.0 24.83 <NA> C <NA>  
## 679 1.0 38.11 <NA> O <NA>  
## 680 1.0 22.95 <NA> C <NA>  
## 681 1.0 19.17 <NA> C <NA>  
## 682 1.0 20.52 <NA> C <NA>  
## 683 1.0 27.67 <NA> N <NA>  
## 684 1.0 21.79 <NA> C <NA>  
## 685 1.0 21.36 <NA> C <NA>  
## 686 1.0 27.98 <NA> O <NA>  
## 687 1.0 18.72 <NA> C <NA>  
## 688 1.0 24.02 <NA> C <NA>  
## 689 1.0 25.75 <NA> C <NA>  
## 690 1.0 26.66 <NA> O <NA>  
## 691 1.0 20.26 <NA> N <NA>  
## 692 1.0 25.28 <NA> N <NA>  
## 693 1.0 17.64 <NA> C <NA>  
## 694 1.0 17.89 <NA> C <NA>  
## 695 1.0 25.23 <NA> O <NA>  
## 696 1.0 20.35 <NA> C <NA>  
## 697 1.0 22.38 <NA> N <NA>  
## 698 1.0 22.19 <NA> C <NA>  
## 699 1.0 15.62 <NA> C <NA>  
## 700 1.0 17.98 <NA> O <NA>  
## 701 1.0 24.08 <NA> C <NA>  
## 702 1.0 34.20 <NA> C <NA>  
## 703 1.0 41.75 <NA> O <NA>  
## 704 1.0 39.06 <NA> O <NA>  
## 705 1.0 15.98 <NA> N <NA>  
## 706 1.0 22.73 <NA> C <NA>  
## 707 1.0 23.86 <NA> C <NA>  
## 708 1.0 33.99 <NA> O <NA>  
## 709 1.0 22.28 <NA> C <NA>  
## 710 1.0 21.31 <NA> N <NA>  
## 711 1.0 16.80 <NA> C <NA>  
## 712 1.0 15.32 <NA> C <NA>  
## 713 1.0 20.89 <NA> O <NA>  
## 714 1.0 10.89 <NA> C <NA>  
## 715 1.0 18.49 <NA> C <NA>  
## 716 1.0 33.23 <NA> S <NA>  
## 717 1.0 16.18 <NA> C <NA>  
## 718 1.0 15.79 <NA> N <NA>  
## 719 1.0 23.25 <NA> C <NA>  
## 720 1.0 30.72 <NA> C <NA>  
## 721 1.0 33.70 <NA> O <NA>  
## 722 1.0 22.15 <NA> C <NA>  
## 723 1.0 36.03 <NA> C <NA>  
## 724 1.0 36.07 <NA> C <NA>  
## 725 1.0 39.56 <NA> C <NA>  
## 726 1.0 37.58 <NA> N <NA>  
## 727 1.0 36.37 <NA> N <NA>  
## 728 1.0 35.95 <NA> C <NA>  
## 729 1.0 33.57 <NA> C <NA>  
## 730 1.0 41.70 <NA> O <NA>  
## 731 1.0 43.10 <NA> C <NA>  
## 732 1.0 56.84 <NA> C <NA>  
## 733 1.0 72.11 <NA> C <NA>  
## 734 1.0 79.50 <NA> O <NA>  
## 735 1.0 76.65 <NA> O <NA>  
## 736 1.0 30.59 <NA> N <NA>  
## 737 1.0 24.42 <NA> C <NA>  
## 738 1.0 23.68 <NA> C <NA>  
## 739 1.0 32.46 <NA> O <NA>  
## 740 1.0 23.91 <NA> C <NA>  
## 741 1.0 22.97 <NA> N <NA>  
## 742 1.0 20.96 <NA> C <NA>  
## 743 1.0 21.24 <NA> C <NA>  
## 744 1.0 34.50 <NA> O <NA>  
## 745 1.0 19.62 <NA> N <NA>  
## 746 1.0 20.00 <NA> C <NA>  
## 747 1.0 22.23 <NA> C <NA>  
## 748 1.0 26.29 <NA> O <NA>  
## 749 1.0 14.37 <NA> C <NA>  
## 750 1.0 20.28 <NA> C <NA>  
## 751 1.0 26.61 <NA> C <NA>  
## 752 1.0 19.51 <NA> C <NA>  
## 753 1.0 22.11 <NA> N <NA>  
## 754 1.0 25.99 <NA> C <NA>  
## 755 1.0 25.65 <NA> C <NA>  
## 756 1.0 24.93 <NA> O <NA>  
## 757 1.0 24.62 <NA> C <NA>  
## 758 1.0 36.20 <NA> C <NA>  
## 759 1.0 41.00 <NA> O <NA>  
## 760 1.0 28.16 <NA> N <NA>  
## 761 1.0 27.03 <NA> N <NA>  
## 762 1.0 24.39 <NA> C <NA>  
## 763 1.0 19.07 <NA> C <NA>  
## 764 1.0 25.97 <NA> O <NA>  
## 765 1.0 22.10 <NA> C <NA>  
## 766 1.0 16.42 <NA> C <NA>  
## 767 1.0 24.02 <NA> C <NA>  
## 768 1.0 19.57 <NA> N <NA>  
## 769 1.0 17.19 <NA> C <NA>  
## 770 1.0 15.75 <NA> C <NA>  
## 771 1.0 22.74 <NA> O <NA>  
## 772 1.0 24.88 <NA> C <NA>  
## 773 1.0 24.98 <NA> C <NA>  
## 774 1.0 43.24 <NA> O <NA>  
## 775 1.0 27.72 <NA> O <NA>  
## 776 1.0 17.82 <NA> N <NA>  
## 777 1.0 12.16 <NA> C <NA>  
## 778 1.0 8.50 <NA> C <NA>  
## 779 1.0 12.46 <NA> O <NA>  
## 780 1.0 11.28 <NA> C <NA>  
## 781 1.0 15.27 <NA> C <NA>  
## 782 1.0 24.66 <NA> C <NA>  
## 783 1.0 19.68 <NA> C <NA>  
## 784 1.0 22.49 <NA> C <NA>  
## 785 1.0 25.60 <NA> C <NA>  
## 786 1.0 25.06 <NA> C <NA>  
## 787 1.0 33.74 <NA> O <NA>  
## 788 1.0 18.01 <NA> N <NA>  
## 789 1.0 17.35 <NA> C <NA>  
## 790 1.0 19.21 <NA> C <NA>  
## 791 1.0 13.86 <NA> O <NA>  
## 792 1.0 18.30 <NA> C <NA>  
## 793 1.0 18.64 <NA> C <NA>  
## 794 1.0 15.06 <NA> C <NA>  
## 795 1.0 18.69 <NA> N <NA>  
## 796 1.0 24.97 <NA> C <NA>  
## 797 1.0 18.25 <NA> C <NA>  
## 798 1.0 23.62 <NA> O <NA>  
## 799 1.0 28.61 <NA> C <NA>  
## 800 1.0 30.93 <NA> C <NA>  
## 801 1.0 34.74 <NA> C <NA>  
## 802 1.0 34.73 <NA> C <NA>  
## 803 1.0 22.27 <NA> N <NA>  
## 804 1.0 14.08 <NA> C <NA>  
## 805 1.0 18.47 <NA> C <NA>  
## 806 1.0 21.54 <NA> O <NA>  
## 807 1.0 21.45 <NA> C <NA>  
## 808 1.0 22.56 <NA> C <NA>  
## 809 1.0 24.65 <NA> C <NA>  
## 810 1.0 19.36 <NA> O <NA>  
## 811 1.0 31.53 <NA> O <NA>  
## 812 1.0 18.92 <NA> N <NA>  
## 813 1.0 22.01 <NA> C <NA>  
## 814 1.0 19.92 <NA> C <NA>  
## 815 1.0 23.47 <NA> O <NA>  
## 816 1.0 22.35 <NA> C <NA>  
## 817 1.0 23.54 <NA> C <NA>  
## 818 1.0 25.40 <NA> C <NA>  
## 819 1.0 30.32 <NA> C <NA>  
## 820 1.0 31.74 <NA> C <NA>  
## 821 1.0 16.97 <NA> C <NA>  
## 822 1.0 27.36 <NA> C <NA>  
## 823 1.0 19.10 <NA> N <NA>  
## 824 1.0 22.26 <NA> C <NA>  
## 825 1.0 25.25 <NA> C <NA>  
## 826 1.0 36.02 <NA> O <NA>  
## 827 1.0 31.65 <NA> C <NA>  
## 828 1.0 35.66 <NA> C <NA>  
## 829 1.0 33.70 <NA> O <NA>  
## 830 1.0 50.40 <NA> O <NA>  
## 831 1.0 25.85 <NA> N <NA>  
## 832 1.0 22.78 <NA> C <NA>  
## 833 1.0 27.86 <NA> C <NA>  
## 834 1.0 36.47 <NA> O <NA>  
## 835 1.0 20.62 <NA> C <NA>  
## 836 1.0 18.76 <NA> C <NA>  
## 837 1.0 18.08 <NA> C <NA>  
## 838 1.0 32.93 <NA> N <NA>  
## 839 1.0 27.47 <NA> C <NA>  
## 840 1.0 24.88 <NA> C <NA>  
## 841 1.0 23.46 <NA> O <NA>  
## 842 1.0 36.49 <NA> C <NA>  
## 843 1.0 36.23 <NA> C <NA>  
## 844 1.0 37.09 <NA> C <NA>  
## 845 1.0 28.58 <NA> N <NA>  
## 846 1.0 30.49 <NA> C <NA>  
## 847 1.0 27.95 <NA> C <NA>  
## 848 1.0 30.96 <NA> O <NA>  
## 849 1.0 35.42 <NA> C <NA>  
## 850 1.0 36.10 <NA> C <NA>  
## 851 1.0 38.70 <NA> O <NA>  
## 852 1.0 34.22 <NA> O <NA>  
## 853 1.0 34.02 <NA> N <NA>  
## 854 1.0 32.02 <NA> C <NA>  
## 855 1.0 26.57 <NA> C <NA>  
## 856 1.0 25.39 <NA> O <NA>  
## 857 1.0 43.95 <NA> C <NA>  
## 858 1.0 52.13 <NA> C <NA>  
## 859 1.0 58.43 <NA> C <NA>  
## 860 1.0 59.64 <NA> O <NA>  
## 861 1.0 55.12 <NA> O <NA>  
## 862 1.0 23.02 <NA> N <NA>  
## 863 1.0 20.90 <NA> C <NA>  
## 864 1.0 24.29 <NA> C <NA>  
## 865 1.0 25.93 <NA> O <NA>  
## 866 1.0 25.86 <NA> C <NA>  
## 867 1.0 24.56 <NA> C <NA>  
## 868 1.0 25.68 <NA> C <NA>  
## 869 1.0 35.21 <NA> C <NA>  
## 870 1.0 28.80 <NA> N <NA>  
## 871 1.0 27.03 <NA> C <NA>  
## 872 1.0 25.43 <NA> C <NA>  
## 873 1.0 32.42 <NA> O <NA>  
## 874 1.0 23.29 <NA> C <NA>  
## 875 1.0 22.29 <NA> C <NA>  
## 876 1.0 25.43 <NA> C <NA>  
## 877 1.0 19.20 <NA> C <NA>  
## 878 1.0 24.16 <NA> N <NA>  
## 879 1.0 23.84 <NA> C <NA>  
## 880 1.0 26.81 <NA> C <NA>  
## 881 1.0 30.82 <NA> O <NA>  
## 882 1.0 21.29 <NA> C <NA>  
## 883 1.0 21.72 <NA> C <NA>  
## 884 1.0 18.79 <NA> C <NA>  
## 885 1.0 35.61 <NA> N <NA>  
## 886 1.0 44.37 <NA> C <NA>  
## 887 1.0 46.52 <NA> C <NA>  
## 888 1.0 50.71 <NA> O <NA>  
## 889 1.0 54.94 <NA> C <NA>  
## 890 1.0 72.81 <NA> C <NA>  
## 891 1.0 79.99 <NA> O <NA>  
## 892 1.0 79.90 <NA> O <NA>  
## 893 1.0 46.17 <NA> N <NA>  
## 894 1.0 42.47 <NA> C <NA>  
## 895 1.0 38.41 <NA> C <NA>  
## 896 1.0 44.02 <NA> O <NA>  
## 897 1.0 44.74 <NA> C <NA>  
## 898 1.0 50.68 <NA> C <NA>  
## 899 1.0 57.44 <NA> C <NA>  
## 900 1.0 62.21 <NA> N <NA>  
## 901 1.0 61.96 <NA> C <NA>  
## 902 1.0 66.73 <NA> N <NA>  
## 903 1.0 60.83 <NA> N <NA>  
## 904 1.0 35.84 <NA> N <NA>  
## 905 1.0 33.48 <NA> C <NA>  
## 906 1.0 38.02 <NA> C <NA>  
## 907 1.0 45.70 <NA> O <NA>  
## 908 1.0 31.88 <NA> C <NA>  
## 909 1.0 28.78 <NA> C <NA>  
## 910 1.0 24.85 <NA> C <NA>  
## 911 1.0 37.67 <NA> C <NA>  
## 912 1.0 40.70 <NA> N <NA>  
## 913 1.0 44.56 <NA> C <NA>  
## 914 1.0 52.05 <NA> C <NA>  
## 915 1.0 52.73 <NA> O <NA>  
## 916 1.0 40.01 <NA> C <NA>  
## 917 1.0 38.17 <NA> C <NA>  
## 918 1.0 37.31 <NA> C <NA>  
## 919 1.0 55.63 <NA> N <NA>  
## 920 1.0 56.67 <NA> C <NA>  
## 921 1.0 58.71 <NA> C <NA>  
## 922 1.0 62.09 <NA> O <NA>  
## 923 1.0 59.98 <NA> N <NA>  
## 924 1.0 60.18 <NA> C <NA>  
## 925 1.0 61.26 <NA> C <NA>  
## 926 1.0 63.95 <NA> O <NA>  
## 927 1.0 58.74 <NA> C <NA>  
## 928 1.0 56.26 <NA> C <NA>  
## 929 1.0 56.51 <NA> C <NA>  
## 930 1.0 54.62 <NA> N <NA>  
## 931 1.0 60.02 <NA> C <NA>  
## 932 1.0 63.19 <NA> N <NA>  
## 933 1.0 57.16 <NA> N <NA>  
## 934 1.0 66.86 <NA> N <NA>  
## 935 1.0 66.62 <NA> C <NA>  
## 936 1.0 62.75 <NA> C <NA>  
## 937 1.0 63.27 <NA> O <NA>  
## 938 1.0 69.46 <NA> C <NA>  
## 939 1.0 74.84 <NA> C <NA>  
## 940 1.0 78.17 <NA> C <NA>  
## 941 1.0 80.81 <NA> N <NA>  
## 942 1.0 79.23 <NA> C <NA>  
## 943 1.0 75.80 <NA> N <NA>  
## 944 1.0 79.30 <NA> N <NA>  
## 945 1.0 59.71 <NA> N <NA>  
## 946 1.0 59.95 <NA> C <NA>  
## 947 1.0 58.01 <NA> C <NA>  
## 948 1.0 54.64 <NA> O <NA>  
## 949 1.0 62.59 <NA> C <NA>  
## 950 1.0 63.31 <NA> C <NA>  
## 951 1.0 58.41 <NA> C <NA>  
## 952 1.0 62.07 <NA> N <NA>  
## 953 1.0 70.81 <NA> C <NA>  
## 954 1.0 73.64 <NA> C <NA>  
## 955 1.0 67.83 <NA> O <NA>  
## 956 1.0 72.91 <NA> C <NA>  
## 957 1.0 76.37 <NA> C <NA>  
## 958 1.0 78.38 <NA> N <NA>  
## 959 1.0 77.84 <NA> C <NA>  
## 960 1.0 75.59 <NA> C <NA>  
## 961 1.0 77.83 <NA> N <NA>  
## 962 1.0 79.04 <NA> N <NA>  
## 963 1.0 88.63 <NA> C <NA>  
## 964 1.0 95.72 <NA> C <NA>  
## 965 1.0 97.84 <NA> O <NA>  
## 966 1.0 88.30 <NA> C <NA>  
## 967 1.0 101.01 <NA> N <NA>  
## 968 1.0 100.11 <NA> C <NA>  
## 969 1.0 97.70 <NA> C <NA>  
## 970 1.0 100.18 <NA> O <NA>  
## 971 1.0 102.27 <NA> C <NA>  
## 972 1.0 102.31 <NA> C <NA>  
## 973 1.0 103.28 <NA> C <NA>  
## 974 1.0 93.37 <NA> N <NA>  
## 975 1.0 86.60 <NA> C <NA>  
## 976 1.0 84.95 <NA> C <NA>  
## 977 1.0 76.21 <NA> O <NA>  
## 978 1.0 84.14 <NA> C <NA>  
## 979 1.0 81.91 <NA> O <NA>  
## 980 1.0 85.52 <NA> N <NA>  
## 981 1.0 85.80 <NA> C <NA>  
## 982 1.0 85.79 <NA> C <NA>  
## 983 1.0 90.38 <NA> O <NA>  
## 984 1.0 81.98 <NA> N <NA>  
## 985 1.0 77.48 <NA> C <NA>  
## 986 1.0 74.18 <NA> C <NA>  
## 987 1.0 71.03 <NA> O <NA>  
## 988 1.0 82.26 <NA> C <NA>  
## 989 1.0 86.49 <NA> C <NA>  
## 990 1.0 88.01 <NA> C <NA>  
## 991 1.0 86.02 <NA> N <NA>  
## 992 1.0 88.71 <NA> C <NA>  
## 993 1.0 95.13 <NA> N <NA>  
## 994 1.0 87.89 <NA> N <NA>  
## 995 1.0 70.85 <NA> N <NA>  
## 996 1.0 68.13 <NA> C <NA>  
## 997 1.0 63.58 <NA> C <NA>  
## 998 1.0 64.70 <NA> O <NA>  
## 999 1.0 65.24 <NA> C <NA>  
## 1000 1.0 69.78 <NA> C <NA>  
## 1001 1.0 67.56 <NA> C <NA>  
## 1002 1.0 59.25 <NA> N <NA>  
## 1003 1.0 52.66 <NA> C <NA>  
## 1004 1.0 47.16 <NA> C <NA>  
## 1005 1.0 44.78 <NA> O <NA>  
## 1006 1.0 51.96 <NA> C <NA>  
## 1007 1.0 53.38 <NA> C <NA>  
## 1008 1.0 48.85 <NA> C <NA>  
## 1009 1.0 54.84 <NA> C <NA>  
## 1010 1.0 48.96 <NA> C <NA>  
## 1011 1.0 54.14 <NA> C <NA>  
## 1012 1.0 52.07 <NA> C <NA>  
## 1013 1.0 55.20 <NA> O <NA>  
## 1014 1.0 44.50 <NA> N <NA>  
## 1015 1.0 45.34 <NA> C <NA>  
## 1016 1.0 47.72 <NA> C <NA>  
## 1017 1.0 44.55 <NA> O <NA>  
## 1018 1.0 41.70 <NA> C <NA>  
## 1019 1.0 42.48 <NA> C <NA>  
## 1020 1.0 43.46 <NA> N <NA>  
## 1021 1.0 40.69 <NA> C <NA>  
## 1022 1.0 48.10 <NA> C <NA>  
## 1023 1.0 44.05 <NA> N <NA>  
## 1024 1.0 49.35 <NA> N <NA>  
## 1025 1.0 52.43 <NA> C <NA>  
## 1026 1.0 60.79 <NA> C <NA>  
## 1027 1.0 67.32 <NA> O <NA>  
## 1028 1.0 54.02 <NA> C <NA>  
## 1029 1.0 55.14 <NA> C <NA>  
## 1030 1.0 48.08 <NA> C <NA>  
## 1031 1.0 63.27 <NA> N <NA>  
## 1032 1.0 60.90 <NA> C <NA>  
## 1033 1.0 60.63 <NA> C <NA>  
## 1034 1.0 65.96 <NA> O <NA>  
## 1035 1.0 61.70 <NA> C <NA>  
## 1036 1.0 67.31 <NA> C <NA>  
## 1037 1.0 78.88 <NA> C <NA>  
## 1038 1.0 80.86 <NA> C <NA>  
## 1039 1.0 81.42 <NA> N <NA>  
## 1040 1.0 60.31 <NA> N <NA>  
## 1041 1.0 62.64 <NA> C <NA>  
## 1042 1.0 64.76 <NA> C <NA>  
## 1043 1.0 67.11 <NA> O <NA>  
## 1044 1.0 60.53 <NA> C <NA>  
## 1045 1.0 60.32 <NA> C <NA>  
## 1046 1.0 57.29 <NA> C <NA>  
## 1047 1.0 60.36 <NA> C <NA>  
## 1048 1.0 52.99 <NA> C <NA>  
## 1049 1.0 56.96 <NA> C <NA>  
## 1050 1.0 56.34 <NA> C <NA>  
## 1051 1.0 69.58 <NA> N <NA>  
## 1052 1.0 72.19 <NA> C <NA>  
## 1053 1.0 68.64 <NA> C <NA>  
## 1054 1.0 70.48 <NA> O <NA>  
## 1055 1.0 79.73 <NA> C <NA>  
## 1056 1.0 83.51 <NA> C <NA>  
## 1057 1.0 87.52 <NA> O <NA>  
## 1058 1.0 82.83 <NA> N <NA>  
## 1059 1.0 67.38 <NA> N <NA>  
## 1060 1.0 66.75 <NA> C <NA>  
## 1061 1.0 64.02 <NA> C <NA>  
## 1062 1.0 68.11 <NA> O <NA>  
## 1063 1.0 72.18 <NA> C <NA>  
## 1064 1.0 71.86 <NA> C <NA>  
## 1065 1.0 67.37 <NA> C <NA>  
## 1066 1.0 58.99 <NA> N <NA>  
## 1067 1.0 58.73 <NA> C <NA>  
## 1068 1.0 62.58 <NA> C <NA>  
## 1069 1.0 59.19 <NA> O <NA>  
## 1070 1.0 54.66 <NA> C <NA>  
## 1071 1.0 54.15 <NA> C <NA>  
## 1072 1.0 58.05 <NA> C <NA>  
## 1073 1.0 69.47 <NA> N <NA>  
## 1074 1.0 74.57 <NA> C <NA>  
## 1075 1.0 73.44 <NA> C <NA>  
## 1076 1.0 72.42 <NA> O <NA>  
## 1077 1.0 80.20 <NA> C <NA>  
## 1078 1.0 82.79 <NA> C <NA>  
## 1079 1.0 89.33 <NA> C <NA>  
## 1080 1.0 96.21 <NA> C <NA>  
## 1081 1.0 99.76 <NA> N <NA>  
## 1082 1.0 77.03 <NA> N <NA>  
## 1083 1.0 79.29 <NA> C <NA>  
## 1084 1.0 79.57 <NA> C <NA>  
## 1085 1.0 77.30 <NA> O <NA>  
## 1086 1.0 79.17 <NA> C <NA>  
## 1087 1.0 76.13 <NA> C <NA>  
## 1088 1.0 80.03 <NA> C <NA>  
## 1089 1.0 77.42 <NA> N <NA>  
## 1090 1.0 79.53 <NA> C <NA>  
## 1091 1.0 78.96 <NA> C <NA>  
## 1092 1.0 74.79 <NA> O <NA>  
## 1093 1.0 81.86 <NA> C <NA>  
## 1094 1.0 85.24 <NA> C <NA>  
## 1095 1.0 83.41 <NA> C <NA>  
## 1096 1.0 76.93 <NA> O <NA>  
## 1097 1.0 85.27 <NA> O <NA>  
## 1098 1.0 79.37 <NA> N <NA>  
## 1099 1.0 76.58 <NA> C <NA>  
## 1100 1.0 75.67 <NA> C <NA>  
## 1101 1.0 77.37 <NA> O <NA>  
## 1102 1.0 72.73 <NA> N <NA>  
## 1103 1.0 66.40 <NA> C <NA>  
## 1104 1.0 64.19 <NA> C <NA>  
## 1105 1.0 64.68 <NA> O <NA>  
## 1106 1.0 63.54 <NA> C <NA>  
## 1107 1.0 56.65 <NA> C <NA>  
## 1108 1.0 61.79 <NA> C <NA>  
## 1109 1.0 71.26 <NA> C <NA>  
## 1110 1.0 74.76 <NA> N <NA>  
## 1111 1.0 60.45 <NA> N <NA>  
## 1112 1.0 64.76 <NA> C <NA>  
## 1113 1.0 65.49 <NA> C <NA>  
## 1114 1.0 65.09 <NA> O <NA>  
## 1115 1.0 63.78 <NA> C <NA>  
## 1116 1.0 62.06 <NA> C <NA>  
## 1117 1.0 58.70 <NA> O <NA>  
## 1118 1.0 59.98 <NA> O <NA>  
## 1119 1.0 67.31 <NA> N <NA>  
## 1120 1.0 70.48 <NA> C <NA>  
## 1121 1.0 74.62 <NA> C <NA>  
## 1122 1.0 79.73 <NA> O <NA>  
## 1123 1.0 64.68 <NA> C <NA>  
## 1124 1.0 67.01 <NA> C <NA>  
## 1125 1.0 62.15 <NA> O <NA>  
## 1126 1.0 63.97 <NA> O <NA>  
## 1127 1.0 78.16 <NA> N <NA>  
## 1128 1.0 74.84 <NA> C <NA>  
## 1129 1.0 73.81 <NA> C <NA>  
## 1130 1.0 78.33 <NA> O <NA>  
## 1131 1.0 73.54 <NA> C <NA>  
## 1132 1.0 73.24 <NA> C <NA>  
## 1133 1.0 68.21 <NA> C <NA>  
## 1134 1.0 72.70 <NA> N <NA>  
## 1135 1.0 70.11 <NA> C <NA>  
## 1136 1.0 72.86 <NA> C <NA>  
## 1137 1.0 72.62 <NA> O <NA>  
## 1138 1.0 62.82 <NA> C <NA>  
## 1139 1.0 62.09 <NA> O <NA>  
## 1140 1.0 63.29 <NA> C <NA>  
## 1141 1.0 72.57 <NA> N <NA>  
## 1142 1.0 74.82 <NA> C <NA>  
## 1143 1.0 74.81 <NA> C <NA>  
## 1144 1.0 76.21 <NA> O <NA>  
## 1145 1.0 75.54 <NA> N <NA>  
## 1146 1.0 78.61 <NA> C <NA>  
## 1147 1.0 76.34 <NA> C <NA>  
## 1148 1.0 74.44 <NA> O <NA>  
## 1149 1.0 80.11 <NA> C <NA>  
## 1150 1.0 88.61 <NA> C <NA>  
## 1151 1.0 92.01 <NA> C <NA>  
## 1152 1.0 93.03 <NA> O <NA>  
## 1153 1.0 95.54 <NA> O <NA>  
## 1154 1.0 76.20 <NA> N <NA>  
## 1155 1.0 78.24 <NA> C <NA>  
## 1156 1.0 75.21 <NA> C <NA>  
## 1157 1.0 75.33 <NA> O <NA>  
## 1158 1.0 83.07 <NA> C <NA>  
## 1159 1.0 87.58 <NA> C <NA>  
## 1160 1.0 86.92 <NA> C <NA>  
## 1161 1.0 82.74 <NA> O <NA>  
## 1162 1.0 87.38 <NA> O <NA>  
## 1163 1.0 69.86 <NA> N <NA>  
## 1164 1.0 66.70 <NA> C <NA>  
## 1165 1.0 67.33 <NA> C <NA>  
## 1166 1.0 68.53 <NA> O <NA>  
## 1167 1.0 62.56 <NA> C <NA>  
## 1168 1.0 50.56 <NA> C <NA>  
## 1169 1.0 46.88 <NA> C <NA>  
## 1170 1.0 44.34 <NA> C <NA>  
## 1171 1.0 67.70 <NA> N <NA>  
## 1172 1.0 66.10 <NA> C <NA>  
## 1173 1.0 62.85 <NA> C <NA>  
## 1174 1.0 53.99 <NA> O <NA>  
## 1175 1.0 68.09 <NA> C <NA>  
## 1176 1.0 72.45 <NA> O <NA>  
## 1177 1.0 68.00 <NA> C <NA>  
## 1178 1.0 63.03 <NA> N <NA>  
## 1179 1.0 67.01 <NA> C <NA>  
## 1180 1.0 66.17 <NA> C <NA>  
## 1181 1.0 63.90 <NA> O <NA>  
## 1182 1.0 68.20 <NA> C <NA>  
## 1183 1.0 68.48 <NA> O <NA>  
## 1184 1.0 71.81 <NA> C <NA>  
## 1185 1.0 66.59 <NA> N <NA>  
## 1186 1.0 72.28 <NA> C <NA>  
## 1187 1.0 73.18 <NA> C <NA>  
## 1188 1.0 68.34 <NA> O <NA>  
## 1189 1.0 79.59 <NA> C <NA>  
## 1190 1.0 93.70 <NA> C <NA>  
## 1191 1.0 99.77 <NA> C <NA>  
## 1192 1.0 103.15 <NA> N <NA>  
## 1193 1.0 105.61 <NA> C <NA>  
## 1194 1.0 105.96 <NA> N <NA>  
## 1195 1.0 108.65 <NA> N <NA>  
## 1196 1.0 78.44 <NA> N <NA>  
## 1197 1.0 80.64 <NA> C <NA>  
## 1198 1.0 75.71 <NA> C <NA>  
## 1199 1.0 71.17 <NA> O <NA>  
## 1200 1.0 89.08 <NA> C <NA>  
## 1201 1.0 97.23 <NA> C <NA>  
## 1202 1.0 104.17 <NA> C <NA>  
## 1203 1.0 106.94 <NA> C <NA>  
## 1204 1.0 109.80 <NA> N <NA>  
## 1205 1.0 73.00 <NA> N <NA>  
## 1206 1.0 68.54 <NA> C <NA>  
## 1207 1.0 62.97 <NA> C <NA>  
## 1208 1.0 65.83 <NA> O <NA>  
## 1209 1.0 74.94 <NA> C <NA>  
## 1210 1.0 76.46 <NA> C <NA>  
## 1211 1.0 78.68 <NA> O <NA>  
## 1212 1.0 79.15 <NA> O <NA>  
## 1213 1.0 54.15 <NA> N <NA>  
## 1214 1.0 43.23 <NA> C <NA>  
## 1215 1.0 42.36 <NA> C <NA>  
## 1216 1.0 43.57 <NA> O <NA>  
## 1217 1.0 49.28 <NA> C <NA>  
## 1218 1.0 50.66 <NA> C <NA>  
## 1219 1.0 43.51 <NA> O <NA>  
## 1220 1.0 51.35 <NA> O <NA>  
## 1221 1.0 47.26 <NA> N <NA>  
## 1222 1.0 51.24 <NA> C <NA>  
## 1223 1.0 44.46 <NA> C <NA>  
## 1224 1.0 43.48 <NA> O <NA>  
## 1225 1.0 61.61 <NA> C <NA>  
## 1226 1.0 72.68 <NA> C <NA>  
## 1227 1.0 83.29 <NA> C <NA>  
## 1228 1.0 86.33 <NA> O <NA>  
## 1229 1.0 85.39 <NA> N <NA>  
## 1230 1.0 41.20 <NA> N <NA>  
## 1231 1.0 45.72 <NA> C <NA>  
## 1232 1.0 48.25 <NA> C <NA>  
## 1233 1.0 50.49 <NA> O <NA>  
## 1234 1.0 52.13 <NA> C <NA>  
## 1235 1.0 57.42 <NA> C <NA>  
## 1236 1.0 62.65 <NA> C <NA>  
## 1237 1.0 59.89 <NA> O <NA>  
## 1238 1.0 67.44 <NA> O <NA>  
## 1239 1.0 56.65 <NA> N <NA>  
## 1240 1.0 61.60 <NA> C <NA>  
## 1241 1.0 57.19 <NA> C <NA>  
## 1242 1.0 52.73 <NA> O <NA>  
## 1243 1.0 76.57 <NA> C <NA>  
## 1244 1.0 94.66 <NA> C <NA>  
## 1245 1.0 103.92 <NA> C <NA>  
## 1246 1.0 107.28 <NA> O <NA>  
## 1247 1.0 105.49 <NA> O <NA>  
## 1248 1.0 53.10 <NA> N <NA>  
## 1249 1.0 45.61 <NA> C <NA>  
## 1250 1.0 43.86 <NA> C <NA>  
## 1251 1.0 49.77 <NA> O <NA>  
## 1252 1.0 42.30 <NA> C <NA>  
## 1253 1.0 56.35 <NA> O <NA>  
## 1254 1.0 42.32 <NA> C <NA>  
## 1255 1.0 45.16 <NA> N <NA>  
## 1256 1.0 42.57 <NA> C <NA>  
## 1257 1.0 42.37 <NA> C <NA>  
## 1258 1.0 46.62 <NA> O <NA>  
## 1259 1.0 39.26 <NA> C <NA>  
## 1260 1.0 31.15 <NA> C <NA>  
## 1261 1.0 40.37 <NA> C <NA>  
## 1262 1.0 42.05 <NA> N <NA>  
## 1263 1.0 41.03 <NA> C <NA>  
## 1264 1.0 39.66 <NA> C <NA>  
## 1265 1.0 40.41 <NA> O <NA>  
## 1266 1.0 38.91 <NA> C <NA>  
## 1267 1.0 42.08 <NA> C <NA>  
## 1268 1.0 39.76 <NA> C <NA>  
## 1269 1.0 34.92 <NA> N <NA>  
## 1270 1.0 37.62 <NA> C <NA>  
## 1271 1.0 38.33 <NA> N <NA>  
## 1272 1.0 38.32 <NA> N <NA>  
## 1273 1.0 41.07 <NA> N <NA>  
## 1274 1.0 41.02 <NA> C <NA>  
## 1275 1.0 42.50 <NA> C <NA>  
## 1276 1.0 49.13 <NA> O <NA>  
## 1277 1.0 45.97 <NA> C <NA>  
## 1278 1.0 58.06 <NA> C <NA>  
## 1279 1.0 75.62 <NA> C <NA>  
## 1280 1.0 81.46 <NA> C <NA>  
## 1281 1.0 82.97 <NA> N <NA>  
## 1282 1.0 37.15 <NA> N <NA>  
## 1283 1.0 33.34 <NA> C <NA>  
## 1284 1.0 35.11 <NA> C <NA>  
## 1285 1.0 35.31 <NA> O <NA>  
## 1286 1.0 36.37 <NA> C <NA>  
## 1287 1.0 47.62 <NA> C <NA>  
## 1288 0.5 40.10 <NA> C <NA>  
## 1289 0.5 36.62 <NA> N <NA>  
## 1290 0.5 32.82 <NA> C <NA>  
## 1291 0.5 30.64 <NA> N <NA>  
## 1292 0.5 28.43 <NA> N <NA>  
## 1293 1.0 30.18 <NA> N <NA>  
## 1294 1.0 19.48 <NA> C <NA>  
## 1295 1.0 26.22 <NA> C <NA>  
## 1296 1.0 31.40 <NA> O <NA>  
## 1297 1.0 28.05 <NA> C <NA>  
## 1298 1.0 26.51 <NA> C <NA>  
## 1299 1.0 18.84 <NA> C <NA>  
## 1300 1.0 17.30 <NA> C <NA>  
## 1301 1.0 30.12 <NA> N <NA>  
## 1302 1.0 34.38 <NA> C <NA>  
## 1303 1.0 30.67 <NA> C <NA>  
## 1304 1.0 34.34 <NA> O <NA>  
## 1305 1.0 38.59 <NA> C <NA>  
## 1306 1.0 47.87 <NA> C <NA>  
## 1307 1.0 40.23 <NA> C <NA>  
## 1308 1.0 27.62 <NA> N <NA>  
## 1309 1.0 33.11 <NA> C <NA>  
## 1310 1.0 36.64 <NA> C <NA>  
## 1311 1.0 32.52 <NA> O <NA>  
## 1312 1.0 40.65 <NA> C <NA>  
## 1313 1.0 66.55 <NA> C <NA>  
## 1314 1.0 79.43 <NA> C <NA>  
## 1315 1.0 83.97 <NA> O <NA>  
## 1316 1.0 87.92 <NA> O <NA>  
## 1317 1.0 31.71 <NA> N <NA>  
## 1318 1.0 25.48 <NA> C <NA>  
## 1319 1.0 24.25 <NA> C <NA>  
## 1320 1.0 24.45 <NA> O <NA>  
## 1321 1.0 21.15 <NA> C <NA>  
## 1322 1.0 16.97 <NA> C <NA>  
## 1323 1.0 10.61 <NA> C <NA>  
## 1324 1.0 18.51 <NA> C <NA>  
## 1325 1.0 9.96 <NA> C <NA>  
## 1326 1.0 18.14 <NA> C <NA>  
## 1327 1.0 14.05 <NA> C <NA>  
## 1328 1.0 21.94 <NA> O <NA>  
## 1329 1.0 26.80 <NA> N <NA>  
## 1330 1.0 29.68 <NA> C <NA>  
## 1331 1.0 35.02 <NA> C <NA>  
## 1332 1.0 40.50 <NA> O <NA>  
## 1333 1.0 31.62 <NA> C <NA>  
## 1334 1.0 26.16 <NA> C <NA>  
## 1335 1.0 34.12 <NA> N <NA>  
## 1336 1.0 28.50 <NA> C <NA>  
## 1337 1.0 34.74 <NA> C <NA>  
## 1338 1.0 37.14 <NA> N <NA>  
## 1339 1.0 30.59 <NA> N <NA>  
## 1340 1.0 40.71 <NA> C <NA>  
## 1341 1.0 40.44 <NA> C <NA>  
## 1342 1.0 38.67 <NA> O <NA>  
## 1343 1.0 48.00 <NA> C <NA>  
## 1344 1.0 64.89 <NA> C <NA>  
## 1345 1.0 72.38 <NA> C <NA>  
## 1346 1.0 78.40 <NA> O <NA>  
## 1347 1.0 72.99 <NA> N <NA>  
## 1348 1.0 39.83 <NA> N <NA>  
## 1349 1.0 32.91 <NA> C <NA>  
## 1350 1.0 28.94 <NA> C <NA>  
## 1351 1.0 32.13 <NA> O <NA>  
## 1352 1.0 34.76 <NA> C <NA>  
## 1353 1.0 37.22 <NA> C <NA>  
## 1354 1.0 49.44 <NA> S <NA>  
## 1355 1.0 51.40 <NA> C <NA>  
## 1356 1.0 22.86 <NA> N <NA>  
## 1357 1.0 24.41 <NA> C <NA>  
## 1358 1.0 27.35 <NA> C <NA>  
## 1359 1.0 35.60 <NA> O <NA>  
## 1360 1.0 26.02 <NA> C <NA>  
## 1361 1.0 32.09 <NA> O <NA>  
## 1362 1.0 30.61 <NA> C <NA>  
## 1363 1.0 25.05 <NA> N <NA>  
## 1364 1.0 19.20 <NA> C <NA>  
## 1365 1.0 13.72 <NA> C <NA>  
## 1366 1.0 22.42 <NA> O <NA>  
## 1367 1.0 22.74 <NA> C <NA>  
## 1368 1.0 13.42 <NA> N <NA>  
## 1369 1.0 15.43 <NA> C <NA>  
## 1370 1.0 22.52 <NA> C <NA>  
## 1371 1.0 24.14 <NA> O <NA>  
## 1372 1.0 8.15 <NA> C <NA>  
## 1373 1.0 10.88 <NA> C <NA>  
## 1374 1.0 12.44 <NA> C <NA>  
## 1375 1.0 21.65 <NA> N <NA>  
## 1376 1.0 19.93 <NA> C <NA>  
## 1377 1.0 22.37 <NA> C <NA>  
## 1378 1.0 23.08 <NA> O <NA>  
## 1379 1.0 18.43 <NA> C <NA>  
## 1380 1.0 19.75 <NA> C <NA>  
## 1381 1.0 22.58 <NA> C <NA>  
## 1382 1.0 14.04 <NA> C <NA>  
## 1383 1.0 24.71 <NA> N <NA>  
## 1384 1.0 20.66 <NA> C <NA>  
## 1385 1.0 20.77 <NA> C <NA>  
## 1386 1.0 27.25 <NA> O <NA>  
## 1387 1.0 21.99 <NA> C <NA>  
## 1388 1.0 18.67 <NA> C <NA>  
## 1389 1.0 26.91 <NA> C <NA>  
## 1390 1.0 30.82 <NA> C <NA>  
## 1391 1.0 19.56 <NA> N <NA>  
## 1392 1.0 12.72 <NA> C <NA>  
## 1393 1.0 15.18 <NA> C <NA>  
## 1394 1.0 18.45 <NA> O <NA>  
## 1395 1.0 15.65 <NA> N <NA>  
## 1396 1.0 21.40 <NA> C <NA>  
## 1397 1.0 19.08 <NA> C <NA>  
## 1398 1.0 22.92 <NA> O <NA>  
## 1399 1.0 19.07 <NA> C <NA>  
## 1400 1.0 24.87 <NA> C <NA>  
## 1401 1.0 17.91 <NA> C <NA>  
## 1402 1.0 23.91 <NA> C <NA>  
## 1403 1.0 18.29 <NA> C <NA>  
## 1404 1.0 33.13 <NA> C <NA>  
## 1405 1.0 28.91 <NA> C <NA>  
## 1406 1.0 34.28 <NA> O <NA>  
## 1407 1.0 18.26 <NA> N <NA>  
## 1408 1.0 18.21 <NA> C <NA>  
## 1409 1.0 22.06 <NA> C <NA>  
## 1410 1.0 27.28 <NA> O <NA>  
## 1411 1.0 14.19 <NA> C <NA>  
## 1412 1.0 17.66 <NA> C <NA>  
## 1413 1.0 18.21 <NA> C <NA>  
## 1414 1.0 13.09 <NA> C <NA>  
## 1415 1.0 12.16 <NA> C <NA>  
## 1416 1.0 11.61 <NA> C <NA>  
## 1417 1.0 12.22 <NA> C <NA>  
## 1418 1.0 21.08 <NA> O <NA>  
## 1419 1.0 22.92 <NA> N <NA>  
## 1420 1.0 26.68 <NA> C <NA>  
## 1421 1.0 29.10 <NA> C <NA>  
## 1422 1.0 34.81 <NA> O <NA>  
## 1423 1.0 23.95 <NA> C <NA>  
## 1424 1.0 37.60 <NA> O <NA>  
## 1425 1.0 36.67 <NA> N <NA>  
## 1426 1.0 34.50 <NA> C <NA>  
## 1427 1.0 25.15 <NA> C <NA>  
## 1428 1.0 29.47 <NA> O <NA>  
## 1429 1.0 39.16 <NA> C <NA>  
## 1430 1.0 53.60 <NA> C <NA>  
## 1431 1.0 59.66 <NA> C <NA>  
## 1432 1.0 62.49 <NA> C <NA>  
## 1433 1.0 57.64 <NA> N <NA>  
## 1434 1.0 28.89 <NA> N <NA>  
## 1435 1.0 25.77 <NA> C <NA>  
## 1436 1.0 26.79 <NA> C <NA>  
## 1437 1.0 31.32 <NA> O <NA>  
## 1438 1.0 25.81 <NA> C <NA>  
## 1439 1.0 22.97 <NA> C <NA>  
## 1440 1.0 29.00 <NA> C <NA>  
## 1441 1.0 30.95 <NA> O <NA>  
## 1442 1.0 39.73 <NA> O <NA>  
## 1443 1.0 28.67 <NA> N <NA>  
## 1444 1.0 26.52 <NA> C <NA>  
## 1445 1.0 30.40 <NA> C <NA>  
## 1446 1.0 29.92 <NA> O <NA>  
## 1447 1.0 27.90 <NA> C <NA>  
## 1448 1.0 35.13 <NA> N <NA>  
## 1449 1.0 36.85 <NA> C <NA>  
## 1450 1.0 34.57 <NA> C <NA>  
## 1451 1.0 36.32 <NA> O <NA>  
## 1452 1.0 42.18 <NA> C <NA>  
## 1453 1.0 63.33 <NA> C <NA>  
## 1454 1.0 71.47 <NA> C <NA>  
## 1455 1.0 70.70 <NA> O <NA>  
## 1456 1.0 70.52 <NA> O <NA>  
## 1457 1.0 31.66 <NA> N <NA>  
## 1458 1.0 31.05 <NA> C <NA>  
## 1459 1.0 37.92 <NA> C <NA>  
## 1460 1.0 42.09 <NA> O <NA>  
## 1461 1.0 40.95 <NA> C <NA>  
## 1462 1.0 43.82 <NA> N <NA>  
## 1463 1.0 39.84 <NA> C <NA>  
## 1464 1.0 40.67 <NA> C <NA>  
## 1465 1.0 40.03 <NA> O <NA>  
## 1466 1.0 45.25 <NA> N <NA>  
## 1467 1.0 48.03 <NA> C <NA>  
## 1468 1.0 45.98 <NA> C <NA>  
## 1469 1.0 49.43 <NA> O <NA>  
## 1470 1.0 51.97 <NA> C <NA>  
## 1471 1.0 54.12 <NA> C <NA>  
## 1472 1.0 50.36 <NA> O <NA>  
## 1473 1.0 57.10 <NA> N <NA>  
## 1474 1.0 38.13 <NA> N <NA>  
## 1475 1.0 23.04 <NA> C <NA>  
## 1476 1.0 24.67 <NA> C <NA>  
## 1477 1.0 29.73 <NA> O <NA>  
## 1478 1.0 20.36 <NA> C <NA>  
## 1479 1.0 23.68 <NA> O <NA>  
## 1480 1.0 27.08 <NA> C <NA>  
## 1481 1.0 25.19 <NA> N <NA>  
## 1482 1.0 29.57 <NA> C <NA>  
## 1483 1.0 24.06 <NA> C <NA>  
## 1484 1.0 33.84 <NA> O <NA>  
## 1485 1.0 39.79 <NA> C <NA>  
## 1486 1.0 58.09 <NA> C <NA>  
## 1487 1.0 80.93 <NA> C <NA>  
## 1488 1.0 86.10 <NA> C <NA>  
## 1489 1.0 87.44 <NA> N <NA>  
## 1490 1.0 26.11 <NA> N <NA>  
## 1491 1.0 23.00 <NA> C <NA>  
## 1492 1.0 24.47 <NA> C <NA>  
## 1493 1.0 27.90 <NA> O <NA>  
## 1494 1.0 20.40 <NA> C <NA>  
## 1495 1.0 15.61 <NA> C <NA>  
## 1496 1.0 14.33 <NA> C <NA>  
## 1497 1.0 26.90 <NA> C <NA>  
## 1498 1.0 15.21 <NA> C <NA>  
## 1499 1.0 22.16 <NA> C <NA>  
## 1500 1.0 21.66 <NA> C <NA>  
## 1501 1.0 30.60 <NA> O <NA>  
## 1502 1.0 20.69 <NA> N <NA>  
## 1503 1.0 23.80 <NA> C <NA>  
## 1504 1.0 17.05 <NA> C <NA>  
## 1505 1.0 22.29 <NA> O <NA>  
## 1506 1.0 26.70 <NA> C <NA>  
## 1507 1.0 24.56 <NA> N <NA>  
## 1508 1.0 26.59 <NA> C <NA>  
## 1509 1.0 29.31 <NA> C <NA>  
## 1510 1.0 33.69 <NA> O <NA>  
## 1511 1.0 35.58 <NA> C <NA>  
## 1512 1.0 44.75 <NA> C <NA>  
## 1513 1.0 51.77 <NA> C <NA>  
## 1514 1.0 57.49 <NA> C <NA>  
## 1515 1.0 65.45 <NA> N <NA>  
## 1516 1.0 27.35 <NA> N <NA>  
## 1517 1.0 25.49 <NA> C <NA>  
## 1518 1.0 23.26 <NA> C <NA>  
## 1519 1.0 28.62 <NA> O <NA>  
## 1520 1.0 27.39 <NA> C <NA>  
## 1521 1.0 22.64 <NA> C <NA>  
## 1522 1.0 32.05 <NA> C <NA>  
## 1523 1.0 28.15 <NA> N <NA>  
## 1524 1.0 23.25 <NA> C <NA>  
## 1525 1.0 16.79 <NA> C <NA>  
## 1526 1.0 20.36 <NA> O <NA>  
## 1527 1.0 32.87 <NA> C <NA>  
## 1528 1.0 35.14 <NA> C <NA>  
## 1529 1.0 46.33 <NA> O <NA>  
## 1530 1.0 43.69 <NA> O <NA>  
## 1531 1.0 19.21 <NA> N <NA>  
## 1532 1.0 19.89 <NA> C <NA>  
## 1533 1.0 27.39 <NA> C <NA>  
## 1534 1.0 30.38 <NA> O <NA>  
## 1535 1.0 31.47 <NA> N <NA>  
## 1536 1.0 32.37 <NA> C <NA>  
## 1537 1.0 33.29 <NA> C <NA>  
## 1538 1.0 43.40 <NA> O <NA>  
## 1539 1.0 28.38 <NA> C <NA>  
## 1540 1.0 22.59 <NA> O <NA>  
## 1541 1.0 25.36 <NA> C <NA>  
## 1542 1.0 29.14 <NA> N <NA>  
## 1543 1.0 30.97 <NA> C <NA>  
## 1544 1.0 34.73 <NA> C <NA>  
## 1545 1.0 31.37 <NA> O <NA>  
## 1546 1.0 15.22 <NA> C <NA>  
## 1547 1.0 20.06 <NA> C <NA>  
## 1548 1.0 20.76 <NA> C <NA>  
## 1549 1.0 30.61 <NA> C <NA>  
## 1550 1.0 43.04 <NA> N <NA>  
## 1551 1.0 41.64 <NA> N <NA>  
## 1552 1.0 42.16 <NA> C <NA>  
## 1553 1.0 33.66 <NA> C <NA>  
## 1554 1.0 32.12 <NA> O <NA>  
## 1555 1.0 52.95 <NA> C <NA>  
## 1556 1.0 52.65 <NA> C <NA>  
## 1557 1.0 44.40 <NA> C <NA>  
## 1558 1.0 29.89 <NA> N <NA>  
## 1559 1.0 29.64 <NA> C <NA>  
## 1560 1.0 30.93 <NA> C <NA>  
## 1561 1.0 24.39 <NA> O <NA>  
## 1562 1.0 32.20 <NA> C <NA>  
## 1563 1.0 34.01 <NA> C <NA>  
## 1564 1.0 30.52 <NA> C <NA>  
## 1565 1.0 33.40 <NA> N <NA>  
## 1566 1.0 29.69 <NA> C <NA>  
## 1567 1.0 33.81 <NA> C <NA>  
## 1568 1.0 31.21 <NA> O <NA>  
## 1569 1.0 28.43 <NA> C <NA>  
## 1570 1.0 32.92 <NA> N <NA>  
## 1571 1.0 33.15 <NA> C <NA>  
## 1572 1.0 32.48 <NA> C <NA>  
## 1573 1.0 41.01 <NA> O <NA>  
## 1574 1.0 36.60 <NA> C <NA>  
## 1575 1.0 41.38 <NA> C <NA>  
## 1576 1.0 48.51 <NA> C <NA>  
## 1577 1.0 53.83 <NA> O <NA>  
## 1578 1.0 56.13 <NA> O <NA>  
## 1579 1.0 30.87 <NA> N <NA>  
## 1580 1.0 26.38 <NA> C <NA>  
## 1581 1.0 27.71 <NA> C <NA>  
## 1582 1.0 29.37 <NA> O <NA>  
## 1583 1.0 27.74 <NA> C <NA>  
## 1584 1.0 28.54 <NA> C <NA>  
## 1585 1.0 16.10 <NA> C <NA>  
## 1586 1.0 23.16 <NA> N <NA>  
## 1587 1.0 23.17 <NA> C <NA>  
## 1588 1.0 30.66 <NA> C <NA>  
## 1589 1.0 36.98 <NA> O <NA>  
## 1590 1.0 25.95 <NA> C <NA>  
## 1591 1.0 37.04 <NA> C <NA>  
## 1592 1.0 53.87 <NA> C <NA>  
## 1593 1.0 68.01 <NA> N <NA>  
## 1594 1.0 75.18 <NA> C <NA>  
## 1595 1.0 73.48 <NA> N <NA>  
## 1596 1.0 78.87 <NA> N <NA>  
## 1597 1.0 36.91 <NA> N <NA>  
## 1598 1.0 29.35 <NA> C <NA>  
## 1599 1.0 26.83 <NA> C <NA>  
## 1600 1.0 31.96 <NA> O <NA>  
## 1601 1.0 35.74 <NA> C <NA>  
## 1602 1.0 32.05 <NA> N <NA>  
## 1603 1.0 32.80 <NA> C <NA>  
## 1604 1.0 36.41 <NA> C <NA>  
## 1605 1.0 37.78 <NA> O <NA>  
## 1606 1.0 37.45 <NA> C <NA>  
## 1607 1.0 40.62 <NA> C <NA>  
## 1608 1.0 51.35 <NA> O <NA>  
## 1609 1.0 42.58 <NA> O <NA>  
## 1610 1.0 30.14 <NA> N <NA>  
## 1611 1.0 25.92 <NA> C <NA>  
## 1612 1.0 32.60 <NA> C <NA>  
## 1613 1.0 38.97 <NA> O <NA>  
## 1614 1.0 20.57 <NA> C <NA>  
## 1615 1.0 20.93 <NA> C <NA>  
## 1616 1.0 21.58 <NA> C <NA>  
## 1617 1.0 21.62 <NA> C <NA>  
## 1618 1.0 39.91 <NA> N <NA>  
## 1619 1.0 38.01 <NA> C <NA>  
## 1620 1.0 41.28 <NA> C <NA>  
## 1621 1.0 46.63 <NA> O <NA>  
## 1622 1.0 41.76 <NA> C <NA>  
## 1623 1.0 52.63 <NA> C <NA>  
## 1624 1.0 58.45 <NA> C <NA>  
## 1625 1.0 53.83 <NA> O <NA>  
## 1626 1.0 63.79 <NA> O <NA>  
## 1627 1.0 42.39 <NA> N <NA>  
## 1628 1.0 45.95 <NA> C <NA>  
## 1629 1.0 47.91 <NA> C <NA>  
## 1630 1.0 51.78 <NA> O <NA>  
## 1631 1.0 54.80 <NA> C <NA>  
## 1632 1.0 66.24 <NA> C <NA>  
## 1633 1.0 75.93 <NA> C <NA>  
## 1634 1.0 77.63 <NA> C <NA>  
## 1635 1.0 75.70 <NA> N <NA>  
## 1636 1.0 49.73 <NA> N <NA>  
## 1637 1.0 44.26 <NA> C <NA>  
## 1638 1.0 43.63 <NA> C <NA>  
## 1639 1.0 46.06 <NA> O <NA>  
## 1640 1.0 41.60 <NA> C <NA>  
## 1641 1.0 35.98 <NA> C <NA>  
## 1642 1.0 42.76 <NA> C <NA>  
## 1643 1.0 38.06 <NA> C <NA>  
## 1644 1.0 44.75 <NA> N <NA>  
## 1645 1.0 44.35 <NA> C <NA>  
## 1646 1.0 52.29 <NA> C <NA>  
## 1647 1.0 47.46 <NA> O <NA>  
## 1648 1.0 30.95 <NA> C <NA>  
## 1649 1.0 26.56 <NA> C <NA>  
## 1650 1.0 28.13 <NA> C <NA>  
## 1651 1.0 22.13 <NA> C <NA>  
## 1652 1.0 59.71 <NA> N <NA>  
## 1653 1.0 70.26 <NA> C <NA>  
## 1654 1.0 78.29 <NA> C <NA>  
## 1655 1.0 83.78 <NA> O <NA>  
## 1656 1.0 79.24 <NA> O <NA>  
## 1657 1.0 38.38 <NA> N <NA>  
## 1658 1.0 26.14 <NA> C <NA>  
## 1659 1.0 23.90 <NA> C <NA>  
## 1660 1.0 20.27 <NA> O <NA>  
## 1661 1.0 31.73 <NA> C <NA>  
## 1662 1.0 35.74 <NA> C <NA>  
## 1663 1.0 39.69 <NA> S <NA>  
## 1664 1.0 39.02 <NA> C <NA>  
## 1665 1.0 16.63 <NA> N <NA>  
## 1666 1.0 16.71 <NA> C <NA>  
## 1667 1.0 20.47 <NA> C <NA>  
## 1668 1.0 21.86 <NA> O <NA>  
## 1669 1.0 27.49 <NA> C <NA>  
## 1670 1.0 29.58 <NA> C <NA>  
## 1671 1.0 39.14 <NA> C <NA>  
## 1672 1.0 45.43 <NA> N <NA>  
## 1673 1.0 43.13 <NA> C <NA>  
## 1674 1.0 32.44 <NA> N <NA>  
## 1675 1.0 44.42 <NA> N <NA>  
## 1676 1.0 19.35 <NA> N <NA>  
## 1677 1.0 15.54 <NA> C <NA>  
## 1678 1.0 15.29 <NA> C <NA>  
## 1679 1.0 18.83 <NA> O <NA>  
## 1680 1.0 20.99 <NA> C <NA>  
## 1681 1.0 17.87 <NA> C <NA>  
## 1682 1.0 22.72 <NA> C <NA>  
## 1683 1.0 14.74 <NA> C <NA>  
## 1684 1.0 19.32 <NA> N <NA>  
## 1685 1.0 20.37 <NA> C <NA>  
## 1686 1.0 19.61 <NA> C <NA>  
## 1687 1.0 19.76 <NA> O <NA>  
## 1688 1.0 28.16 <NA> C <NA>  
## 1689 1.0 17.10 <NA> C <NA>  
## 1690 1.0 28.24 <NA> C <NA>  
## 1691 1.0 12.08 <NA> C <NA>  
## 1692 1.0 18.91 <NA> N <NA>  
## 1693 1.0 17.08 <NA> C <NA>  
## 1694 1.0 17.45 <NA> C <NA>  
## 1695 1.0 23.44 <NA> O <NA>  
## 1696 1.0 18.00 <NA> C <NA>  
## 1697 1.0 22.57 <NA> C <NA>  
## 1698 1.0 19.07 <NA> C <NA>  
## 1699 1.0 30.32 <NA> C <NA>  
## 1700 1.0 18.86 <NA> N <NA>  
## 1701 1.0 19.01 <NA> C <NA>  
## 1702 1.0 18.47 <NA> C <NA>  
## 1703 1.0 27.19 <NA> O <NA>  
## 1704 1.0 11.00 <NA> C <NA>  
## 1705 1.0 21.73 <NA> C <NA>  
## 1706 1.0 13.75 <NA> C <NA>  
## 1707 1.0 15.07 <NA> C <NA>  
## 1708 1.0 22.28 <NA> N <NA>  
## 1709 1.0 16.74 <NA> C <NA>  
## 1710 1.0 17.47 <NA> C <NA>  
## 1711 1.0 20.37 <NA> O <NA>  
## 1712 1.0 27.03 <NA> N <NA>  
## 1713 1.0 20.81 <NA> C <NA>  
## 1714 1.0 22.77 <NA> C <NA>  
## 1715 1.0 27.45 <NA> O <NA>  
## 1716 1.0 19.89 <NA> C <NA>  
## 1717 1.0 28.81 <NA> N <NA>  
## 1718 1.0 20.62 <NA> C <NA>  
## 1719 1.0 27.01 <NA> C <NA>  
## 1720 1.0 26.39 <NA> O <NA>  
## 1721 1.0 23.29 <NA> C <NA>  
## 1722 1.0 16.08 <NA> C <NA>  
## 1723 1.0 22.28 <NA> C <NA>  
## 1724 1.0 29.20 <NA> N <NA>  
## 1725 1.0 25.54 <NA> C <NA>  
## 1726 1.0 28.56 <NA> C <NA>  
## 1727 1.0 34.54 <NA> O <NA>  
## 1728 1.0 27.46 <NA> N <NA>  
## 1729 1.0 27.71 <NA> C <NA>  
## 1730 1.0 30.55 <NA> C <NA>  
## 1731 1.0 42.55 <NA> O <NA>  
## 1732 1.0 21.94 <NA> C <NA>  
## 1733 1.0 35.60 <NA> N <NA>  
## 1734 1.0 30.26 <NA> C <NA>  
## 1735 1.0 31.17 <NA> C <NA>  
## 1736 1.0 31.14 <NA> O <NA>  
## 1737 1.0 29.63 <NA> N <NA>  
## 1738 1.0 29.44 <NA> C <NA>  
## 1739 1.0 31.56 <NA> C <NA>  
## 1740 1.0 32.16 <NA> O <NA>  
## 1741 1.0 23.69 <NA> C <NA>  
## 1742 1.0 23.01 <NA> C <NA>  
## 1743 1.0 24.28 <NA> C <NA>  
## 1744 1.0 31.21 <NA> C <NA>  
## 1745 1.0 34.69 <NA> N <NA>  
## 1746 1.0 31.86 <NA> N <NA>  
## 1747 1.0 32.28 <NA> C <NA>  
## 1748 1.0 35.03 <NA> C <NA>  
## 1749 1.0 46.12 <NA> O <NA>  
## 1750 1.0 39.78 <NA> N <NA>  
## 1751 1.0 37.59 <NA> C <NA>  
## 1752 1.0 33.26 <NA> C <NA>  
## 1753 1.0 45.76 <NA> O <NA>  
## 1754 1.0 40.67 <NA> C <NA>  
## 1755 1.0 46.97 <NA> O <NA>  
## 1756 1.0 34.81 <NA> C <NA>  
## 1757 1.0 27.58 <NA> N <NA>  
## 1758 1.0 26.78 <NA> C <NA>  
## 1759 1.0 24.01 <NA> C <NA>  
## 1760 1.0 24.42 <NA> O <NA>  
## 1761 1.0 30.56 <NA> C <NA>  
## 1762 1.0 37.68 <NA> C <NA>  
## 1763 1.0 37.25 <NA> C <NA>  
## 1764 1.0 33.80 <NA> O <NA>  
## 1765 1.0 40.37 <NA> N <NA>  
## 1766 1.0 24.84 <NA> N <NA>  
## 1767 1.0 27.10 <NA> C <NA>  
## 1768 1.0 27.26 <NA> C <NA>  
## 1769 1.0 33.13 <NA> O <NA>  
## 1770 1.0 23.33 <NA> C <NA>  
## 1771 1.0 27.99 <NA> N <NA>  
## 1772 1.0 26.97 <NA> C <NA>  
## 1773 1.0 24.78 <NA> C <NA>  
## 1774 1.0 27.05 <NA> O <NA>  
## 1775 1.0 36.42 <NA> C <NA>  
## 1776 1.0 42.94 <NA> C <NA>  
## 1777 1.0 50.81 <NA> C <NA>  
## 1778 1.0 51.24 <NA> O <NA>  
## 1779 1.0 51.74 <NA> N <NA>  
## 1780 1.0 24.96 <NA> N <NA>  
## 1781 1.0 25.39 <NA> C <NA>  
## 1782 1.0 26.16 <NA> C <NA>  
## 1783 1.0 29.88 <NA> O <NA>  
## 1784 1.0 29.34 <NA> C <NA>  
## 1785 1.0 34.74 <NA> C <NA>  
## 1786 1.0 37.15 <NA> C <NA>  
## 1787 1.0 31.98 <NA> C <NA>  
## 1788 1.0 41.73 <NA> C <NA>  
## 1789 1.0 30.62 <NA> C <NA>  
## 1790 1.0 39.05 <NA> C <NA>  
## 1791 1.0 25.42 <NA> N <NA>  
## 1792 1.0 20.88 <NA> C <NA>  
## 1793 1.0 18.82 <NA> C <NA>  
## 1794 1.0 23.31 <NA> O <NA>  
## 1795 1.0 20.41 <NA> C <NA>  
## 1796 1.0 21.67 <NA> C <NA>  
## 1797 1.0 17.32 <NA> C <NA>  
## 1798 1.0 21.59 <NA> C <NA>  
## 1799 1.0 20.84 <NA> N <NA>  
## 1800 1.0 21.04 <NA> C <NA>  
## 1801 1.0 24.85 <NA> C <NA>  
## 1802 1.0 21.56 <NA> O <NA>  
## 1803 1.0 21.42 <NA> C <NA>  
## 1804 1.0 13.40 <NA> C <NA>  
## 1805 1.0 28.59 <NA> S <NA>  
## 1806 1.0 27.97 <NA> C <NA>  
## 1807 1.0 23.59 <NA> N <NA>  
## 1808 1.0 32.65 <NA> C <NA>  
## 1809 1.0 31.66 <NA> C <NA>  
## 1810 1.0 33.22 <NA> O <NA>  
## 1811 1.0 39.43 <NA> C <NA>  
## 1812 1.0 52.77 <NA> C <NA>  
## 1813 1.0 55.84 <NA> C <NA>  
## 1814 1.0 58.06 <NA> O <NA>  
## 1815 1.0 66.12 <NA> O <NA>  
## 1816 1.0 32.63 <NA> N <NA>  
## 1817 1.0 35.63 <NA> C <NA>  
## 1818 1.0 36.20 <NA> C <NA>  
## 1819 1.0 41.36 <NA> O <NA>  
## 1820 1.0 43.91 <NA> C <NA>  
## 1821 1.0 53.92 <NA> C <NA>  
## 1822 1.0 60.12 <NA> C <NA>  
## 1823 1.0 61.26 <NA> C <NA>  
## 1824 1.0 63.66 <NA> N <NA>  
## 1825 1.0 37.20 <NA> N <NA>  
## 1826 1.0 27.87 <NA> C <NA>  
## 1827 1.0 25.86 <NA> C <NA>  
## 1828 1.0 35.14 <NA> O <NA>  
## 1829 1.0 27.44 <NA> C <NA>  
## 1830 1.0 34.51 <NA> C <NA>  
## 1831 1.0 36.36 <NA> C <NA>  
## 1832 1.0 32.21 <NA> C <NA>  
## 1833 1.0 34.94 <NA> C <NA>  
## 1834 1.0 37.47 <NA> C <NA>  
## 1835 1.0 40.00 <NA> C <NA>  
## 1836 1.0 54.33 <NA> O <NA>  
## 1837 1.0 23.04 <NA> N <NA>  
## 1838 1.0 21.20 <NA> C <NA>  
## 1839 1.0 25.31 <NA> C <NA>  
## 1840 1.0 28.30 <NA> O <NA>  
## 1841 1.0 22.09 <NA> N <NA>  
## 1842 1.0 14.88 <NA> C <NA>  
## 1843 1.0 15.21 <NA> C <NA>  
## 1844 1.0 16.28 <NA> O <NA>  
## 1845 1.0 13.60 <NA> C <NA>  
## 1846 1.0 16.26 <NA> C <NA>  
## 1847 1.0 10.35 <NA> C <NA>  
## 1848 1.0 7.58 <NA> C <NA>  
## 1849 1.0 13.64 <NA> N <NA>  
## 1850 1.0 11.23 <NA> C <NA>  
## 1851 1.0 18.17 <NA> C <NA>  
## 1852 1.0 24.15 <NA> O <NA>  
## 1853 1.0 10.30 <NA> C <NA>  
## 1854 1.0 8.34 <NA> C <NA>  
## 1855 1.0 7.56 <NA> C <NA>  
## 1856 1.0 21.44 <NA> N <NA>  
## 1857 1.0 24.04 <NA> C <NA>  
## 1858 1.0 23.79 <NA> C <NA>  
## 1859 1.0 23.53 <NA> O <NA>  
## 1860 1.0 28.91 <NA> C <NA>  
## 1861 1.0 31.80 <NA> C <NA>  
## 1862 1.0 37.79 <NA> C <NA>  
## 1863 1.0 40.82 <NA> O <NA>  
## 1864 1.0 42.77 <NA> N <NA>  
## 1865 1.0 29.44 <NA> N <NA>  
## 1866 1.0 20.40 <NA> C <NA>  
## 1867 1.0 18.98 <NA> C <NA>  
## 1868 1.0 22.80 <NA> O <NA>  
## 1869 1.0 30.75 <NA> C <NA>  
## 1870 1.0 23.69 <NA> C <NA>  
## 1871 1.0 36.03 <NA> C <NA>  
## 1872 1.0 28.59 <NA> C <NA>  
## 1873 1.0 24.77 <NA> N <NA>  
## 1874 1.0 23.92 <NA> C <NA>  
## 1875 1.0 26.47 <NA> C <NA>  
## 1876 1.0 29.50 <NA> O <NA>  
## 1877 1.0 23.08 <NA> C <NA>  
## 1878 1.0 31.57 <NA> O <NA>  
## 1879 1.0 28.16 <NA> N <NA>  
## 1880 1.0 29.64 <NA> C <NA>  
## 1881 1.0 32.16 <NA> C <NA>  
## 1882 1.0 41.41 <NA> O <NA>  
## 1883 1.0 31.83 <NA> C <NA>  
## 1884 1.0 32.46 <NA> O <NA>  
## 1885 1.0 28.07 <NA> C <NA>  
## 1886 1.0 24.68 <NA> N <NA>  
## 1887 1.0 24.39 <NA> C <NA>  
## 1888 1.0 30.73 <NA> C <NA>  
## 1889 1.0 34.51 <NA> O <NA>  
## 1890 1.0 35.80 <NA> N <NA>  
## 1891 1.0 38.02 <NA> C <NA>  
## 1892 1.0 35.80 <NA> C <NA>  
## 1893 1.0 39.72 <NA> O <NA>  
## 1894 1.0 37.07 <NA> C <NA>  
## 1895 1.0 42.09 <NA> C <NA>  
## 1896 1.0 43.99 <NA> O <NA>  
## 1897 1.0 44.21 <NA> O <NA>  
## 1898 1.0 41.46 <NA> N <NA>  
## 1899 1.0 40.87 <NA> C <NA>  
## 1900 1.0 38.85 <NA> C <NA>  
## 1901 1.0 34.14 <NA> O <NA>  
## 1902 1.0 39.20 <NA> C <NA>  
## 1903 1.0 35.24 <NA> C <NA>  
## 1904 1.0 44.57 <NA> S <NA>  
## 1905 1.0 41.16 <NA> C <NA>  
## 1906 1.0 42.33 <NA> N <NA>  
## 1907 1.0 45.53 <NA> C <NA>  
## 1908 1.0 45.85 <NA> C <NA>  
## 1909 1.0 56.61 <NA> O <NA>  
## 1910 1.0 49.35 <NA> C <NA>  
## 1911 1.0 52.56 <NA> C <NA>  
## 1912 1.0 58.92 <NA> C <NA>  
## 1913 1.0 52.37 <NA> C <NA>  
## 1914 1.0 45.36 <NA> N <NA>  
## 1915 1.0 42.39 <NA> C <NA>  
## 1916 1.0 41.63 <NA> C <NA>  
## 1917 1.0 48.24 <NA> O <NA>  
## 1918 1.0 41.71 <NA> C <NA>  
## 1919 1.0 45.39 <NA> C <NA>  
## 1920 1.0 51.19 <NA> C <NA>  
## 1921 1.0 58.60 <NA> N <NA>  
## 1922 1.0 61.21 <NA> C <NA>  
## 1923 1.0 62.74 <NA> N <NA>  
## 1924 1.0 63.10 <NA> N <NA>  
## 1925 1.0 35.52 <NA> N <NA>  
## 1926 1.0 45.45 <NA> C <NA>  
## 1927 1.0 52.61 <NA> C <NA>  
## 1928 1.0 62.24 <NA> O <NA>  
## 1929 1.0 51.54 <NA> C <NA>  
## 1930 1.0 52.92 <NA> N <NA>  
## 1931 1.0 51.67 <NA> C <NA>  
## 1932 1.0 52.97 <NA> C <NA>  
## 1933 1.0 50.30 <NA> O <NA>  
## 1934 1.0 52.36 <NA> C <NA>  
## 1935 1.0 56.23 <NA> N <NA>  
## 1936 1.0 56.95 <NA> C <NA>  
## 1937 1.0 63.03 <NA> C <NA>  
## 1938 1.0 70.03 <NA> O <NA>  
## 1939 1.0 53.04 <NA> C <NA>  
## 1940 1.0 52.64 <NA> C <NA>  
## 1941 1.0 52.14 <NA> C <NA>  
## 1942 1.0 69.30 <NA> N <NA>  
## 1943 1.0 73.31 <NA> C <NA>  
## 1944 1.0 72.81 <NA> C <NA>  
## 1945 1.0 72.57 <NA> O <NA>  
## 1946 1.0 78.94 <NA> C <NA>  
## 1947 1.0 81.30 <NA> C <NA>  
## 1948 1.0 80.58 <NA> C <NA>  
## 1949 1.0 74.80 <NA> C <NA>  
## 1950 1.0 61.65 <NA> N <NA>  
## 1951 1.0 75.64 <NA> N <NA>  
## 1952 1.0 78.97 <NA> C <NA>  
## 1953 1.0 75.30 <NA> C <NA>  
## 1954 1.0 76.48 <NA> O <NA>  
## 1955 1.0 85.04 <NA> C <NA>  
## 1956 1.0 97.95 <NA> O <NA>  
## 1957 1.0 70.12 <NA> N <NA>  
## 1958 1.0 64.76 <NA> C <NA>  
## 1959 1.0 63.86 <NA> C <NA>  
## 1960 1.0 65.89 <NA> O <NA>  
## 1961 1.0 61.41 <NA> N <NA>  
## 1962 1.0 55.63 <NA> C <NA>  
## 1963 1.0 55.12 <NA> C <NA>  
## 1964 1.0 54.12 <NA> O <NA>  
## 1965 1.0 57.25 <NA> C <NA>  
## 1966 1.0 55.11 <NA> O <NA>  
## 1967 1.0 56.78 <NA> N <NA>  
## 1968 1.0 54.14 <NA> C <NA>  
## 1969 1.0 49.30 <NA> C <NA>  
## 1970 1.0 45.15 <NA> O <NA>  
## 1971 1.0 60.09 <NA> C <NA>  
## 1972 1.0 69.81 <NA> C <NA>  
## 1973 1.0 77.89 <NA> C <NA>  
## 1974 1.0 81.52 <NA> O <NA>  
## 1975 1.0 79.87 <NA> O <NA>  
## 1976 1.0 46.63 <NA> N <NA>  
## 1977 1.0 40.59 <NA> C <NA>  
## 1978 1.0 41.55 <NA> C <NA>  
## 1979 1.0 44.88 <NA> O <NA>  
## 1980 1.0 38.48 <NA> C <NA>  
## 1981 1.0 46.01 <NA> C <NA>  
## 1982 1.0 49.64 <NA> C <NA>  
## 1983 1.0 44.28 <NA> C <NA>  
## 1984 1.0 39.11 <NA> N <NA>  
## 1985 1.0 36.89 <NA> C <NA>  
## 1986 1.0 40.06 <NA> C <NA>  
## 1987 1.0 39.11 <NA> O <NA>  
## 1988 1.0 45.15 <NA> N <NA>  
## 1989 1.0 48.77 <NA> C <NA>  
## 1990 1.0 45.79 <NA> C <NA>  
## 1991 1.0 48.46 <NA> O <NA>  
## 1992 1.0 61.79 <NA> C <NA>  
## 1993 1.0 75.73 <NA> C <NA>  
## 1994 1.0 87.90 <NA> C <NA>  
## 1995 1.0 93.57 <NA> C <NA>  
## 1996 1.0 93.53 <NA> N <NA>  
## 1997 1.0 38.94 <NA> N <NA>  
## 1998 1.0 40.56 <NA> C <NA>  
## 1999 1.0 39.82 <NA> C <NA>  
## 2000 1.0 46.21 <NA> O <NA>  
## 2001 1.0 41.55 <NA> C <NA>  
## 2002 1.0 49.76 <NA> C <NA>  
## 2003 1.0 59.04 <NA> C <NA>  
## 2004 1.0 68.60 <NA> O <NA>  
## 2005 1.0 63.25 <NA> N <NA>  
## 2006 1.0 35.46 <NA> N <NA>  
## 2007 1.0 37.77 <NA> C <NA>  
## 2008 1.0 33.54 <NA> C <NA>  
## 2009 1.0 34.18 <NA> O <NA>  
## 2010 1.0 36.19 <NA> C <NA>  
## 2011 1.0 37.20 <NA> N <NA>  
## 2012 1.0 39.67 <NA> C <NA>  
## 2013 1.0 45.94 <NA> C <NA>  
## 2014 1.0 52.82 <NA> O <NA>  
## 2015 1.0 37.90 <NA> C <NA>  
## 2016 1.0 43.72 <NA> C <NA>  
## 2017 1.0 54.39 <NA> C <NA>  
## 2018 1.0 59.30 <NA> C <NA>  
## 2019 1.0 55.97 <NA> N <NA>  
## 2020 1.0 51.15 <NA> N <NA>  
## 2021 1.0 53.21 <NA> C <NA>  
## 2022 1.0 51.51 <NA> C <NA>  
## 2023 1.0 59.71 <NA> O <NA>  
## 2024 1.0 63.72 <NA> C <NA>  
## 2025 1.0 67.01 <NA> C <NA>  
## 2026 1.0 73.02 <NA> O <NA>  
## 2027 1.0 70.56 <NA> O <NA>  
## 2028 1.0 47.89 <NA> N <NA>  
## 2029 1.0 40.57 <NA> C <NA>  
## 2030 1.0 37.94 <NA> C <NA>  
## 2031 1.0 35.40 <NA> O <NA>  
## 2032 1.0 36.84 <NA> C <NA>  
## 2033 1.0 36.20 <NA> C <NA>  
## 2034 1.0 48.04 <NA> C <NA>  
## 2035 1.0 37.29 <NA> C <NA>  
## 2036 1.0 37.71 <NA> N <NA>  
## 2037 1.0 39.53 <NA> C <NA>  
## 2038 1.0 40.51 <NA> C <NA>  
## 2039 1.0 44.01 <NA> O <NA>  
## 2040 1.0 46.72 <NA> C <NA>  
## 2041 1.0 43.52 <NA> C <NA>  
## 2042 1.0 56.93 <NA> S <NA>  
## 2043 1.0 41.03 <NA> C <NA>  
## 2044 1.0 45.48 <NA> N <NA>  
## 2045 1.0 45.81 <NA> C <NA>  
## 2046 1.0 46.85 <NA> C <NA>  
## 2047 1.0 56.39 <NA> O <NA>  
## 2048 1.0 52.24 <NA> C <NA>  
## 2049 1.0 62.30 <NA> C <NA>  
## 2050 1.0 63.02 <NA> O <NA>  
## 2051 1.0 58.36 <NA> O <NA>  
## 2052 1.0 43.59 <NA> N <NA>  
## 2053 1.0 36.05 <NA> C <NA>  
## 2054 1.0 38.73 <NA> C <NA>  
## 2055 1.0 43.28 <NA> O <NA>  
## 2056 1.0 35.95 <NA> C <NA>  
## 2057 1.0 39.60 <NA> N <NA>  
## 2058 1.0 38.73 <NA> C <NA>  
## 2059 1.0 40.86 <NA> C <NA>  
## 2060 1.0 45.91 <NA> O <NA>  
## 2061 1.0 41.31 <NA> N <NA>  
## 2062 1.0 41.52 <NA> C <NA>  
## 2063 1.0 44.61 <NA> C <NA>  
## 2064 1.0 47.51 <NA> O <NA>  
## 2065 1.0 44.58 <NA> C <NA>  
## 2066 1.0 48.61 <NA> C <NA>  
## 2067 1.0 65.20 <NA> C <NA>  
## 2068 1.0 80.57 <NA> C <NA>  
## 2069 1.0 91.10 <NA> N <NA>  
## 2070 1.0 42.50 <NA> N <NA>  
## 2071 1.0 41.31 <NA> C <NA>  
## 2072 1.0 37.94 <NA> C <NA>  
## 2073 1.0 34.91 <NA> O <NA>  
## 2074 1.0 49.79 <NA> C <NA>  
## 2075 1.0 59.35 <NA> C <NA>  
## 2076 1.0 64.46 <NA> C <NA>  
## 2077 1.0 64.39 <NA> C <NA>  
## 2078 1.0 34.61 <NA> N <NA>  
## 2079 1.0 38.09 <NA> C <NA>  
## 2080 1.0 40.55 <NA> C <NA>  
## 2081 1.0 44.62 <NA> O <NA>  
## 2082 1.0 37.16 <NA> C <NA>  
## 2083 1.0 29.31 <NA> C <NA>  
## 2084 1.0 38.74 <NA> C <NA>  
## 2085 1.0 36.37 <NA> N <NA>  
## 2086 1.0 36.94 <NA> C <NA>  
## 2087 1.0 33.91 <NA> C <NA>  
## 2088 1.0 40.02 <NA> O <NA>  
## 2089 1.0 33.40 <NA> C <NA>  
## 2090 1.0 55.59 <NA> O <NA>  
## 2091 1.0 37.63 <NA> C <NA>  
## 2092 1.0 34.59 <NA> N <NA>  
## 2093 1.0 35.88 <NA> C <NA>  
## 2094 1.0 35.79 <NA> C <NA>  
## 2095 1.0 37.13 <NA> O <NA>  
## 2096 1.0 38.64 <NA> C <NA>  
## 2097 1.0 42.76 <NA> C <NA>  
## 2098 1.0 46.43 <NA> O <NA>  
## 2099 1.0 39.22 <NA> O <NA>  
## 2100 1.0 40.63 <NA> N <NA>  
## 2101 1.0 44.10 <NA> C <NA>  
## 2102 1.0 43.04 <NA> C <NA>  
## 2103 1.0 43.66 <NA> O <NA>  
## 2104 1.0 53.46 <NA> C <NA>  
## 2105 1.0 66.83 <NA> C <NA>  
## 2106 1.0 68.64 <NA> C <NA>  
## 2107 1.0 56.54 <NA> O <NA>  
## 2108 1.0 75.34 <NA> O <NA>  
## 2109 1.0 39.81 <NA> N <NA>  
## 2110 1.0 36.69 <NA> C <NA>  
## 2111 1.0 32.24 <NA> C <NA>  
## 2112 1.0 39.83 <NA> O <NA>  
## 2113 1.0 37.51 <NA> C <NA>  
## 2114 1.0 39.18 <NA> C <NA>  
## 2115 1.0 35.96 <NA> C <NA>  
## 2116 1.0 39.71 <NA> C <NA>  
## 2117 1.0 31.53 <NA> N <NA>  
## 2118 1.0 28.90 <NA> C <NA>  
## 2119 1.0 26.39 <NA> C <NA>  
## 2120 1.0 36.03 <NA> O <NA>  
## 2121 1.0 25.85 <NA> C <NA>  
## 2122 1.0 18.87 <NA> C <NA>  
## 2123 1.0 20.43 <NA> C <NA>  
## 2124 1.0 27.67 <NA> N <NA>  
## 2125 1.0 28.83 <NA> C <NA>  
## 2126 1.0 34.16 <NA> C <NA>  
## 2127 1.0 40.01 <NA> O <NA>  
## 2128 1.0 25.22 <NA> C <NA>  
## 2129 1.0 33.61 <NA> C <NA>  
## 2130 1.0 18.19 <NA> C <NA>  
## 2131 1.0 30.27 <NA> C <NA>  
## 2132 1.0 34.42 <NA> N <NA>  
## 2133 1.0 28.31 <NA> C <NA>  
## 2134 1.0 30.69 <NA> C <NA>  
## 2135 1.0 26.97 <NA> O <NA>  
## 2136 1.0 35.50 <NA> C <NA>  
## 2137 1.0 29.19 <NA> N <NA>  
## 2138 1.0 23.30 <NA> C <NA>  
## 2139 1.0 25.91 <NA> C <NA>  
## 2140 1.0 33.61 <NA> O <NA>  
## 2141 1.0 23.87 <NA> C <NA>  
## 2142 1.0 31.16 <NA> C <NA>  
## 2143 1.0 27.64 <NA> C <NA>  
## 2144 1.0 28.83 <NA> C <NA>  
## 2145 1.0 23.17 <NA> N <NA>  
## 2146 1.0 20.83 <NA> C <NA>  
## 2147 1.0 24.96 <NA> C <NA>  
## 2148 1.0 32.02 <NA> O <NA>  
## 2149 1.0 12.87 <NA> C <NA>  
## 2150 1.0 14.23 <NA> C <NA>  
## 2151 1.0 7.72 <NA> C <NA>  
## 2152 1.0 34.47 <NA> N <NA>  
## 2153 1.0 35.09 <NA> C <NA>  
## 2154 1.0 34.20 <NA> C <NA>  
## 2155 1.0 37.93 <NA> O <NA>  
## 2156 1.0 30.26 <NA> C <NA>  
## 2157 1.0 45.18 <NA> C <NA>  
## 2158 1.0 61.91 <NA> C <NA>  
## 2159 1.0 69.18 <NA> C <NA>  
## 2160 1.0 74.35 <NA> N <NA>  
## 2161 1.0 36.78 <NA> N <NA>  
## 2162 1.0 39.16 <NA> C <NA>  
## 2163 1.0 46.87 <NA> C <NA>  
## 2164 1.0 46.47 <NA> O <NA>  
## 2165 1.0 41.49 <NA> C <NA>  
## 2166 1.0 58.36 <NA> C <NA>  
## 2167 1.0 69.37 <NA> C <NA>  
## 2168 1.0 73.73 <NA> O <NA>  
## 2169 1.0 77.04 <NA> O <NA>  
## 2170 1.0 43.11 <NA> N <NA>  
## 2171 1.0 38.85 <NA> C <NA>  
## 2172 1.0 38.23 <NA> C <NA>  
## 2173 1.0 40.20 <NA> O <NA>  
## 2174 1.0 38.85 <NA> C <NA>  
## 2175 1.0 40.51 <NA> C <NA>  
## 2176 1.0 43.33 <NA> C <NA>  
## 2177 1.0 36.20 <NA> N <NA>  
## 2178 1.0 41.57 <NA> C <NA>  
## 2179 1.0 41.12 <NA> N <NA>  
## 2180 1.0 54.93 <NA> N <NA>  
## 2181 1.0 33.63 <NA> N <NA>  
## 2182 1.0 31.19 <NA> C <NA>  
## 2183 1.0 33.65 <NA> C <NA>  
## 2184 1.0 36.92 <NA> O <NA>  
## 2185 1.0 28.59 <NA> C <NA>  
## 2186 1.0 22.46 <NA> C <NA>  
## 2187 1.0 19.29 <NA> C <NA>  
## 2188 1.0 24.69 <NA> C <NA>  
## 2189 1.0 41.51 <NA> N <NA>  
## 2190 1.0 53.03 <NA> C <NA>  
## 2191 1.0 54.85 <NA> C <NA>  
## 2192 1.0 56.75 <NA> O <NA>  
## 2193 1.0 54.46 <NA> C <NA>  
## 2194 1.0 49.53 <NA> N <NA>  
## 2195 1.0 40.59 <NA> C <NA>  
## 2196 1.0 41.99 <NA> C <NA>  
## 2197 1.0 39.59 <NA> O <NA>  
## 2198 1.0 32.24 <NA> C <NA>  
## 2199 1.0 36.69 <NA> C <NA>  
## 2200 1.0 48.86 <NA> C <NA>  
## 2201 1.0 46.32 <NA> O <NA>  
## 2202 1.0 59.42 <NA> N <NA>  
## 2203 1.0 47.26 <NA> N <NA>  
## 2204 1.0 48.42 <NA> C <NA>  
## 2205 1.0 45.42 <NA> C <NA>  
## 2206 1.0 37.41 <NA> O <NA>  
## 2207 1.0 60.78 <NA> C <NA>  
## 2208 1.0 73.50 <NA> C <NA>  
## 2209 1.0 83.98 <NA> C <NA>  
## 2210 1.0 88.37 <NA> O <NA>  
## 2211 1.0 85.81 <NA> O <NA>  
## 2212 1.0 43.26 <NA> N <NA>  
## 2213 1.0 40.02 <NA> C <NA>  
## 2214 1.0 43.91 <NA> C <NA>  
## 2215 1.0 45.27 <NA> O <NA>  
## 2216 1.0 31.81 <NA> C <NA>  
## 2217 1.0 39.08 <NA> C <NA>  
## 2218 1.0 50.36 <NA> O <NA>  
## 2219 1.0 39.60 <NA> O <NA>  
## 2220 1.0 37.15 <NA> N <NA>  
## 2221 1.0 36.92 <NA> C <NA>  
## 2222 1.0 41.32 <NA> C <NA>  
## 2223 1.0 45.23 <NA> O <NA>  
## 2224 1.0 23.54 <NA> C <NA>  
## 2225 1.0 27.71 <NA> S <NA>  
## 2226 1.0 51.22 <NA> N <NA>  
## 2227 1.0 56.27 <NA> C <NA>  
## 2228 1.0 53.19 <NA> C <NA>  
## 2229 1.0 59.17 <NA> O <NA>  
## 2230 1.0 68.07 <NA> C <NA>  
## 2231 1.0 82.76 <NA> C <NA>  
## 2232 1.0 98.32 <NA> C <NA>  
## 2233 1.0 108.68 <NA> N <NA>  
## 2234 1.0 114.92 <NA> C <NA>  
## 2235 1.0 116.25 <NA> N <NA>  
## 2236 1.0 116.82 <NA> N <NA>  
## 2237 1.0 46.04 <NA> N <NA>  
## 2238 1.0 39.56 <NA> C <NA>  
## 2239 1.0 29.25 <NA> C <NA>  
## 2240 1.0 22.30 <NA> O <NA>  
## 2241 1.0 47.27 <NA> C <NA>  
## 2242 1.0 48.82 <NA> C <NA>  
## 2243 1.0 54.28 <NA> O <NA>  
## 2244 1.0 50.66 <NA> N <NA>  
## 2245 1.0 26.08 <NA> N <NA>  
## 2246 1.0 22.02 <NA> C <NA>  
## 2247 1.0 14.66 <NA> C <NA>  
## 2248 1.0 19.39 <NA> O <NA>  
## 2249 1.0 20.47 <NA> N <NA>  
## 2250 1.0 18.93 <NA> C <NA>  
## 2251 1.0 20.64 <NA> C <NA>  
## 2252 1.0 27.80 <NA> O <NA>  
## 2253 1.0 18.72 <NA> C <NA>  
## 2254 1.0 26.25 <NA> C <NA>  
## 2255 1.0 25.55 <NA> C <NA>  
## 2256 1.0 25.31 <NA> C <NA>  
## 2257 1.0 26.89 <NA> C <NA>  
## 2258 1.0 34.18 <NA> C <NA>  
## 2259 1.0 36.07 <NA> C <NA>  
## 2260 1.0 16.38 <NA> N <NA>  
## 2261 1.0 16.49 <NA> C <NA>  
## 2262 1.0 13.99 <NA> C <NA>  
## 2263 1.0 13.15 <NA> O <NA>  
## 2264 1.0 16.35 <NA> C <NA>  
## 2265 1.0 20.33 <NA> C <NA>  
## 2266 1.0 12.87 <NA> C <NA>  
## 2267 1.0 17.86 <NA> C <NA>  
## 2268 1.0 17.48 <NA> N <NA>  
## 2269 1.0 22.73 <NA> C <NA>  
## 2270 1.0 22.98 <NA> C <NA>  
## 2271 1.0 22.35 <NA> O <NA>  
## 2272 1.0 19.21 <NA> C <NA>  
## 2273 1.0 19.94 <NA> C <NA>  
## 2274 1.0 16.00 <NA> C <NA>  
## 2275 1.0 21.47 <NA> C <NA>  
## 2276 1.0 27.25 <NA> N <NA>  
## 2277 1.0 27.85 <NA> C <NA>  
## 2278 1.0 26.30 <NA> C <NA>  
## 2279 1.0 28.72 <NA> O <NA>  
## 2280 1.0 32.44 <NA> C <NA>  
## 2281 1.0 32.92 <NA> C <NA>  
## 2282 1.0 32.19 <NA> O <NA>  
## 2283 1.0 43.25 <NA> O <NA>  
## 2284 1.0 27.55 <NA> N <NA>  
## 2285 1.0 23.06 <NA> C <NA>  
## 2286 1.0 26.83 <NA> C <NA>  
## 2287 1.0 25.59 <NA> O <NA>  
## 2288 1.0 25.87 <NA> N <NA>  
## 2289 1.0 15.48 <NA> C <NA>  
## 2290 1.0 17.56 <NA> C <NA>  
## 2291 1.0 19.06 <NA> O <NA>  
## 2292 1.0 18.43 <NA> C <NA>  
## 2293 1.0 20.09 <NA> C <NA>  
## 2294 1.0 24.63 <NA> C <NA>  
## 2295 1.0 26.54 <NA> C <NA>  
## 2296 1.0 23.20 <NA> C <NA>  
## 2297 1.0 19.79 <NA> C <NA>  
## 2298 1.0 19.41 <NA> C <NA>  
## 2299 1.0 17.11 <NA> N <NA>  
## 2300 1.0 19.21 <NA> C <NA>  
## 2301 1.0 17.63 <NA> C <NA>  
## 2302 1.0 19.75 <NA> O <NA>  
## 2303 1.0 13.07 <NA> C <NA>  
## 2304 1.0 17.24 <NA> C <NA>  
## 2305 1.0 13.33 <NA> C <NA>  
## 2306 1.0 14.15 <NA> N <NA>  
## 2307 1.0 14.98 <NA> C <NA>  
## 2308 1.0 23.25 <NA> C <NA>  
## 2309 1.0 27.61 <NA> O <NA>  
## 2310 1.0 16.92 <NA> C <NA>  
## 2311 1.0 18.39 <NA> C <NA>  
## 2312 1.0 20.24 <NA> C <NA>  
## 2313 1.0 36.94 <NA> N <NA>  
## 2314 1.0 44.77 <NA> C <NA>  
## 2315 1.0 55.78 <NA> N <NA>  
## 2316 1.0 47.18 <NA> N <NA>  
## 2317 1.0 23.36 <NA> N <NA>  
## 2318 1.0 22.11 <NA> C <NA>  
## 2319 1.0 18.51 <NA> C <NA>  
## 2320 1.0 26.92 <NA> O <NA>  
## 2321 1.0 16.65 <NA> C <NA>  
## 2322 1.0 26.01 <NA> O <NA>  
## 2323 1.0 15.36 <NA> C <NA>  
## 2324 1.0 22.76 <NA> N <NA>  
## 2325 1.0 22.61 <NA> C <NA>  
## 2326 1.0 20.46 <NA> C <NA>  
## 2327 1.0 25.53 <NA> O <NA>  
## 2328 1.0 21.30 <NA> C <NA>  
## 2329 1.0 25.68 <NA> C <NA>  
## 2330 1.0 20.03 <NA> C <NA>  
## 2331 1.0 21.56 <NA> C <NA>  
## 2332 1.0 20.46 <NA> N <NA>  
## 2333 1.0 15.59 <NA> C <NA>  
## 2334 1.0 15.46 <NA> C <NA>  
## 2335 1.0 24.15 <NA> O <NA>  
## 2336 1.0 21.86 <NA> C <NA>  
## 2337 1.0 18.39 <NA> C <NA>  
## 2338 1.0 18.14 <NA> C <NA>  
## 2339 1.0 18.16 <NA> N <NA>  
## 2340 1.0 13.43 <NA> C <NA>  
## 2341 1.0 19.74 <NA> C <NA>  
## 2342 1.0 28.70 <NA> O <NA>  
## 2343 1.0 10.13 <NA> C <NA>  
## 2344 1.0 8.94 <NA> C <NA>  
## 2345 1.0 4.64 <NA> C <NA>  
## 2346 1.0 13.75 <NA> O <NA>  
## 2347 1.0 5.23 <NA> N <NA>  
## 2348 1.0 20.76 <NA> N <NA>  
## 2349 1.0 15.10 <NA> C <NA>  
## 2350 1.0 19.17 <NA> C <NA>  
## 2351 1.0 22.68 <NA> O <NA>  
## 2352 1.0 14.53 <NA> C <NA>  
## 2353 1.0 19.13 <NA> N <NA>  
## 2354 1.0 21.38 <NA> C <NA>  
## 2355 1.0 12.12 <NA> C <NA>  
## 2356 1.0 19.89 <NA> O <NA>  
## 2357 1.0 35.93 <NA> C <NA>  
## 2358 1.0 43.23 <NA> C <NA>  
## 2359 1.0 45.04 <NA> O <NA>  
## 2360 1.0 55.68 <NA> O <NA>  
## 2361 1.0 15.34 <NA> N <NA>  
## 2362 1.0 15.68 <NA> C <NA>  
## 2363 1.0 26.27 <NA> C <NA>  
## 2364 1.0 31.08 <NA> O <NA>  
## 2365 1.0 18.87 <NA> C <NA>  
## 2366 1.0 28.12 <NA> N <NA>  
## 2367 1.0 18.64 <NA> C <NA>  
## 2368 1.0 21.62 <NA> C <NA>  
## 2369 1.0 21.88 <NA> O <NA>  
## 2370 1.0 21.88 <NA> C <NA>  
## 2371 1.0 23.19 <NA> C <NA>  
## 2372 1.0 30.11 <NA> S <NA>  
## 2373 1.0 26.50 <NA> C <NA>  
## 2374 1.0 18.93 <NA> N <NA>  
## 2375 1.0 20.41 <NA> C <NA>  
## 2376 1.0 25.63 <NA> C <NA>  
## 2377 1.0 28.85 <NA> O <NA>  
## 2378 1.0 22.45 <NA> C <NA>  
## 2379 1.0 37.74 <NA> C <NA>  
## 2380 1.0 39.30 <NA> C <NA>  
## 2381 1.0 51.18 <NA> C <NA>  
## 2382 1.0 62.04 <NA> N <NA>  
## 2383 1.0 32.24 <NA> N <NA>  
## 2384 1.0 27.39 <NA> C <NA>  
## 2385 1.0 23.66 <NA> C <NA>  
## 2386 1.0 39.15 <NA> O <NA>  
## 2387 1.0 31.20 <NA> C <NA>  
## 2388 1.0 42.50 <NA> C <NA>  
## 2389 1.0 47.68 <NA> C <NA>  
## 2390 1.0 49.30 <NA> O <NA>  
## 2391 1.0 58.97 <NA> O <NA>  
## 2392 1.0 19.28 <NA> N <NA>  
## 2393 1.0 16.75 <NA> C <NA>  
## 2394 1.0 18.40 <NA> C <NA>  
## 2395 1.0 27.04 <NA> O <NA>  
## 2396 1.0 15.23 <NA> C <NA>  
## 2397 1.0 22.75 <NA> N <NA>  
## 2398 1.0 20.38 <NA> C <NA>  
## 2399 1.0 23.56 <NA> C <NA>  
## 2400 1.0 27.58 <NA> O <NA>  
## 2401 1.0 21.94 <NA> N <NA>  
## 2402 1.0 17.98 <NA> C <NA>  
## 2403 1.0 19.64 <NA> C <NA>  
## 2404 1.0 28.81 <NA> O <NA>  
## 2405 1.0 23.42 <NA> C <NA>  
## 2406 1.0 16.57 <NA> C <NA>  
## 2407 1.0 16.00 <NA> C <NA>  
## 2408 1.0 20.63 <NA> C <NA>  
## 2409 1.0 20.82 <NA> N <NA>  
## 2410 1.0 24.17 <NA> C <NA>  
## 2411 1.0 20.93 <NA> C <NA>  
## 2412 1.0 24.13 <NA> O <NA>  
## 2413 1.0 39.85 <NA> C <NA>  
## 2414 1.0 55.23 <NA> C <NA>  
## 2415 1.0 60.74 <NA> O <NA>  
## 2416 1.0 59.19 <NA> N <NA>  
## 2417 1.0 19.01 <NA> N <NA>  
## 2418 1.0 20.87 <NA> C <NA>  
## 2419 1.0 20.36 <NA> C <NA>  
## 2420 1.0 24.77 <NA> O <NA>  
## 2421 1.0 16.16 <NA> C <NA>  
## 2422 1.0 14.90 <NA> C <NA>  
## 2423 1.0 24.05 <NA> C <NA>  
## 2424 1.0 22.66 <NA> N <NA>  
## 2425 1.0 23.76 <NA> C <NA>  
## 2426 1.0 22.93 <NA> C <NA>  
## 2427 1.0 27.60 <NA> O <NA>  
## 2428 1.0 29.51 <NA> C <NA>  
## 2429 1.0 28.18 <NA> C <NA>  
## 2430 1.0 33.52 <NA> O <NA>  
## 2431 1.0 35.50 <NA> O <NA>  
## 2432 1.0 17.46 <NA> N <NA>  
## 2433 1.0 17.75 <NA> C <NA>  
## 2434 1.0 17.91 <NA> C <NA>  
## 2435 1.0 22.58 <NA> O <NA>  
## 2436 1.0 25.29 <NA> C <NA>  
## 2437 1.0 27.69 <NA> C <NA>  
## 2438 1.0 39.16 <NA> C <NA>  
## 2439 1.0 24.86 <NA> C <NA>  
## 2440 1.0 33.85 <NA> C <NA>  
## 2441 1.0 31.01 <NA> C <NA>  
## 2442 1.0 34.85 <NA> C <NA>  
## 2443 1.0 43.04 <NA> O <NA>  
## 2444 1.0 20.63 <NA> N <NA>  
## 2445 1.0 18.09 <NA> C <NA>  
## 2446 1.0 19.17 <NA> C <NA>  
## 2447 1.0 19.67 <NA> O <NA>  
## 2448 1.0 16.64 <NA> C <NA>  
## 2449 1.0 23.02 <NA> C <NA>  
## 2450 1.0 8.07 <NA> C <NA>  
## 2451 1.0 23.09 <NA> N <NA>  
## 2452 1.0 22.63 <NA> C <NA>  
## 2453 1.0 19.82 <NA> C <NA>  
## 2454 1.0 23.26 <NA> O <NA>  
## 2455 1.0 21.04 <NA> C <NA>  
## 2456 1.0 24.06 <NA> C <NA>  
## 2457 1.0 18.27 <NA> C <NA>  
## 2458 1.0 21.28 <NA> C <NA>  
## 2459 1.0 25.04 <NA> N <NA>  
## 2460 1.0 25.96 <NA> C <NA>  
## 2461 1.0 19.21 <NA> C <NA>  
## 2462 1.0 20.42 <NA> O <NA>  
## 2463 1.0 23.15 <NA> C <NA>  
## 2464 1.0 30.09 <NA> C <NA>  
## 2465 1.0 31.64 <NA> C <NA>  
## 2466 1.0 27.45 <NA> O <NA>  
## 2467 1.0 43.35 <NA> O <NA>  
## 2468 1.0 18.44 <NA> N <NA>  
## 2469 1.0 22.02 <NA> C <NA>  
## 2470 1.0 18.29 <NA> C <NA>  
## 2471 1.0 26.70 <NA> O <NA>  
## 2472 1.0 23.30 <NA> C <NA>  
## 2473 1.0 32.34 <NA> C <NA>  
## 2474 1.0 24.74 <NA> C <NA>  
## 2475 1.0 31.22 <NA> C <NA>  
## 2476 1.0 27.11 <NA> C <NA>  
## 2477 1.0 21.56 <NA> C <NA>  
## 2478 1.0 35.13 <NA> C <NA>  
## 2479 1.0 24.29 <NA> N <NA>  
## 2480 1.0 25.71 <NA> C <NA>  
## 2481 1.0 23.65 <NA> C <NA>  
## 2482 1.0 29.01 <NA> O <NA>  
## 2483 1.0 33.25 <NA> C <NA>  
## 2484 1.0 37.23 <NA> C <NA>  
## 2485 1.0 41.30 <NA> O <NA>  
## 2486 1.0 43.61 <NA> O <NA>  
## 2487 1.0 23.54 <NA> N <NA>  
## 2488 1.0 23.72 <NA> C <NA>  
## 2489 1.0 34.24 <NA> C <NA>  
## 2490 1.0 37.81 <NA> O <NA>  
## 2491 1.0 21.05 <NA> C <NA>  
## 2492 1.0 20.50 <NA> C <NA>  
## 2493 1.0 22.09 <NA> C <NA>  
## 2494 1.0 36.62 <NA> N <NA>  
## 2495 1.0 30.84 <NA> C <NA>  
## 2496 1.0 22.56 <NA> C <NA>  
## 2497 1.0 25.67 <NA> O <NA>  
## 2498 1.0 38.02 <NA> C <NA>  
## 2499 1.0 35.90 <NA> C <NA>  
## 2500 1.0 38.49 <NA> C <NA>  
## 2501 1.0 23.34 <NA> N <NA>  
## 2502 1.0 26.25 <NA> C <NA>  
## 2503 1.0 27.19 <NA> C <NA>  
## 2504 1.0 32.50 <NA> O <NA>  
## 2505 1.0 36.64 <NA> C <NA>  
## 2506 1.0 42.07 <NA> C <NA>  
## 2507 1.0 48.74 <NA> O <NA>  
## 2508 1.0 51.52 <NA> O <NA>  
## 2509 1.0 31.23 <NA> N <NA>  
## 2510 1.0 27.88 <NA> C <NA>  
## 2511 1.0 23.57 <NA> C <NA>  
## 2512 1.0 29.01 <NA> O <NA>  
## 2513 1.0 38.23 <NA> C <NA>  
## 2514 1.0 48.35 <NA> C <NA>  
## 2515 1.0 59.17 <NA> C <NA>  
## 2516 1.0 62.46 <NA> O <NA>  
## 2517 1.0 62.43 <NA> O <NA>  
## 2518 1.0 23.60 <NA> N <NA>  
## 2519 1.0 21.09 <NA> C <NA>  
## 2520 1.0 28.76 <NA> C <NA>  
## 2521 1.0 34.80 <NA> O <NA>  
## 2522 1.0 22.57 <NA> C <NA>  
## 2523 1.0 28.59 <NA> C <NA>  
## 2524 1.0 32.18 <NA> C <NA>  
## 2525 1.0 35.82 <NA> C <NA>  
## 2526 1.0 32.33 <NA> N <NA>  
## 2527 1.0 30.08 <NA> C <NA>  
## 2528 1.0 29.92 <NA> C <NA>  
## 2529 1.0 35.31 <NA> O <NA>  
## 2530 1.0 27.21 <NA> C <NA>  
## 2531 1.0 14.84 <NA> C <NA>  
## 2532 1.0 21.76 <NA> C <NA>  
## 2533 1.0 17.85 <NA> C <NA>  
## 2534 1.0 28.75 <NA> N <NA>  
## 2535 1.0 29.83 <NA> C <NA>  
## 2536 1.0 30.54 <NA> C <NA>  
## 2537 1.0 35.28 <NA> O <NA>  
## 2538 1.0 25.58 <NA> C <NA>  
## 2539 1.0 25.46 <NA> C <NA>  
## 2540 1.0 23.15 <NA> C <NA>  
## 2541 1.0 39.93 <NA> N <NA>  
## 2542 1.0 43.15 <NA> C <NA>  
## 2543 1.0 45.06 <NA> C <NA>  
## 2544 1.0 49.07 <NA> O <NA>  
## 2545 1.0 52.80 <NA> C <NA>  
## 2546 1.0 68.65 <NA> C <NA>  
## 2547 1.0 75.70 <NA> O <NA>  
## 2548 1.0 70.34 <NA> O <NA>  
## 2549 1.0 46.71 <NA> N <NA>  
## 2550 1.0 43.75 <NA> C <NA>  
## 2551 1.0 43.35 <NA> C <NA>  
## 2552 1.0 49.53 <NA> O <NA>  
## 2553 1.0 40.12 <NA> C <NA>  
## 2554 1.0 53.67 <NA> C <NA>  
## 2555 1.0 65.49 <NA> C <NA>  
## 2556 1.0 71.35 <NA> N <NA>  
## 2557 1.0 73.79 <NA> C <NA>  
## 2558 1.0 76.27 <NA> N <NA>  
## 2559 1.0 72.98 <NA> N <NA>  
## 2560 1.0 41.72 <NA> N <NA>  
## 2561 1.0 37.45 <NA> C <NA>  
## 2562 1.0 44.66 <NA> C <NA>  
## 2563 1.0 46.88 <NA> O <NA>  
## 2564 1.0 35.36 <NA> C <NA>  
## 2565 1.0 33.27 <NA> C <NA>  
## 2566 1.0 43.76 <NA> C <NA>  
## 2567 1.0 31.87 <NA> C <NA>  
## 2568 1.0 47.48 <NA> N <NA>  
## 2569 1.0 49.74 <NA> C <NA>  
## 2570 1.0 54.55 <NA> C <NA>  
## 2571 1.0 53.08 <NA> O <NA>  
## 2572 1.0 41.99 <NA> C <NA>  
## 2573 1.0 35.57 <NA> C <NA>  
## 2574 1.0 26.84 <NA> C <NA>  
## 2575 1.0 51.76 <NA> N <NA>  
## 2576 1.0 55.61 <NA> C <NA>  
## 2577 1.0 56.92 <NA> C <NA>  
## 2578 1.0 60.89 <NA> O <NA>  
## 2579 1.0 58.19 <NA> N <NA>  
## 2580 1.0 56.03 <NA> C <NA>  
## 2581 1.0 55.56 <NA> C <NA>  
## 2582 1.0 57.78 <NA> O <NA>  
## 2583 1.0 51.91 <NA> C <NA>  
## 2584 1.0 53.93 <NA> C <NA>  
## 2585 1.0 57.17 <NA> C <NA>  
## 2586 1.0 62.65 <NA> N <NA>  
## 2587 1.0 67.87 <NA> C <NA>  
## 2588 1.0 63.19 <NA> N <NA>  
## 2589 1.0 69.37 <NA> N <NA>  
## 2590 1.0 56.11 <NA> N <NA>  
## 2591 1.0 54.98 <NA> C <NA>  
## 2592 1.0 54.77 <NA> C <NA>  
## 2593 1.0 47.77 <NA> O <NA>  
## 2594 1.0 52.49 <NA> C <NA>  
## 2595 1.0 50.71 <NA> C <NA>  
## 2596 1.0 56.38 <NA> C <NA>  
## 2597 1.0 63.83 <NA> N <NA>  
## 2598 1.0 66.35 <NA> C <NA>  
## 2599 1.0 63.58 <NA> N <NA>  
## 2600 1.0 68.17 <NA> N <NA>  
## 2601 1.0 53.94 <NA> N <NA>  
## 2602 1.0 54.91 <NA> C <NA>  
## 2603 1.0 53.81 <NA> C <NA>  
## 2604 1.0 42.06 <NA> O <NA>  
## 2605 1.0 56.88 <NA> C <NA>  
## 2606 1.0 54.19 <NA> C <NA>  
## 2607 1.0 61.33 <NA> C <NA>  
## 2608 1.0 61.63 <NA> N <NA>  
## 2609 1.0 66.46 <NA> C <NA>  
## 2610 1.0 68.50 <NA> C <NA>  
## 2611 1.0 60.94 <NA> O <NA>  
## 2612 1.0 70.75 <NA> C <NA>  
## 2613 1.0 76.26 <NA> C <NA>  
## 2614 1.0 78.19 <NA> N <NA>  
## 2615 1.0 76.26 <NA> C <NA>  
## 2616 1.0 81.07 <NA> C <NA>  
## 2617 1.0 77.04 <NA> N <NA>  
## 2618 1.0 76.05 <NA> N <NA>  
## 2619 1.0 84.52 <NA> C <NA>  
## 2620 1.0 89.57 <NA> C <NA>  
## 2621 1.0 93.25 <NA> O <NA>  
## 2622 1.0 81.88 <NA> C <NA>  
## 2623 1.0 92.28 <NA> N <NA>  
## 2624 1.0 91.87 <NA> C <NA>  
## 2625 1.0 91.45 <NA> C <NA>  
## 2626 1.0 90.80 <NA> O <NA>  
## 2627 1.0 93.23 <NA> C <NA>  
## 2628 1.0 89.99 <NA> C <NA>  
## 2629 1.0 92.09 <NA> C <NA>  
## 2630 1.0 91.21 <NA> N <NA>  
## 2631 1.0 89.20 <NA> C <NA>  
## 2632 1.0 90.09 <NA> C <NA>  
## 2633 1.0 85.30 <NA> O <NA>  
## 2634 1.0 88.62 <NA> C <NA>  
## 2635 1.0 79.96 <NA> O <NA>  
## 2636 1.0 91.51 <NA> N <NA>  
## 2637 1.0 94.90 <NA> C <NA>  
## 2638 1.0 97.82 <NA> C <NA>  
## 2639 1.0 102.80 <NA> O <NA>  
## 2640 1.0 96.26 <NA> N <NA>  
## 2641 1.0 91.83 <NA> C <NA>  
## 2642 1.0 85.72 <NA> C <NA>  
## 2643 1.0 86.15 <NA> O <NA>  
## 2644 1.0 96.66 <NA> C <NA>  
## 2645 1.0 98.30 <NA> C <NA>  
## 2646 1.0 101.06 <NA> C <NA>  
## 2647 1.0 105.07 <NA> N <NA>  
## 2648 1.0 106.81 <NA> C <NA>  
## 2649 1.0 108.74 <NA> N <NA>  
## 2650 1.0 107.48 <NA> N <NA>  
## 2651 1.0 78.51 <NA> N <NA>  
## 2652 1.0 73.90 <NA> C <NA>  
## 2653 1.0 70.16 <NA> C <NA>  
## 2654 1.0 72.77 <NA> O <NA>  
## 2655 1.0 76.20 <NA> C <NA>  
## 2656 1.0 82.52 <NA> C <NA>  
## 2657 1.0 71.04 <NA> C <NA>  
## 2658 1.0 62.51 <NA> N <NA>  
## 2659 1.0 54.04 <NA> C <NA>  
## 2660 1.0 51.16 <NA> C <NA>  
## 2661 1.0 45.47 <NA> O <NA>  
## 2662 1.0 56.02 <NA> C <NA>  
## 2663 1.0 54.00 <NA> C <NA>  
## 2664 1.0 58.76 <NA> C <NA>  
## 2665 1.0 50.22 <NA> C <NA>  
## 2666 1.0 61.15 <NA> C <NA>  
## 2667 1.0 58.26 <NA> C <NA>  
## 2668 1.0 62.07 <NA> C <NA>  
## 2669 1.0 63.76 <NA> O <NA>  
## 2670 1.0 47.06 <NA> N <NA>  
## 2671 1.0 47.83 <NA> C <NA>  
## 2672 1.0 51.63 <NA> C <NA>  
## 2673 1.0 53.61 <NA> O <NA>  
## 2674 1.0 45.75 <NA> C <NA>  
## 2675 1.0 44.95 <NA> C <NA>  
## 2676 1.0 40.58 <NA> N <NA>  
## 2677 1.0 44.56 <NA> C <NA>  
## 2678 1.0 35.83 <NA> C <NA>  
## 2679 1.0 40.61 <NA> N <NA>  
## 2680 1.0 55.41 <NA> N <NA>  
## 2681 1.0 57.09 <NA> C <NA>  
## 2682 1.0 58.35 <NA> C <NA>  
## 2683 1.0 57.47 <NA> O <NA>  
## 2684 1.0 51.17 <NA> C <NA>  
## 2685 1.0 40.67 <NA> C <NA>  
## 2686 1.0 46.00 <NA> C <NA>  
## 2687 1.0 59.68 <NA> N <NA>  
## 2688 1.0 62.89 <NA> C <NA>  
## 2689 1.0 63.42 <NA> C <NA>  
## 2690 1.0 65.69 <NA> O <NA>  
## 2691 1.0 70.20 <NA> C <NA>  
## 2692 1.0 79.02 <NA> C <NA>  
## 2693 1.0 85.61 <NA> C <NA>  
## 2694 1.0 90.38 <NA> C <NA>  
## 2695 1.0 91.26 <NA> N <NA>  
## 2696 1.0 61.23 <NA> N <NA>  
## 2697 1.0 62.34 <NA> C <NA>  
## 2698 1.0 64.89 <NA> C <NA>  
## 2699 1.0 70.95 <NA> O <NA>  
## 2700 1.0 68.26 <NA> C <NA>  
## 2701 1.0 80.10 <NA> C <NA>  
## 2702 1.0 81.46 <NA> C <NA>  
## 2703 1.0 88.93 <NA> C <NA>  
## 2704 1.0 80.79 <NA> C <NA>  
## 2705 1.0 88.64 <NA> C <NA>  
## 2706 1.0 89.82 <NA> C <NA>  
## 2707 1.0 66.65 <NA> N <NA>  
## 2708 1.0 70.15 <NA> C <NA>  
## 2709 1.0 67.29 <NA> C <NA>  
## 2710 1.0 70.07 <NA> O <NA>  
## 2711 1.0 79.26 <NA> C <NA>  
## 2712 1.0 85.40 <NA> C <NA>  
## 2713 1.0 86.47 <NA> O <NA>  
## 2714 1.0 90.13 <NA> N <NA>  
## 2715 1.0 62.01 <NA> N <NA>  
## 2716 1.0 61.94 <NA> C <NA>  
## 2717 1.0 63.38 <NA> C <NA>  
## 2718 1.0 61.88 <NA> O <NA>  
## 2719 1.0 61.87 <NA> C <NA>  
## 2720 1.0 64.63 <NA> C <NA>  
## 2721 1.0 58.80 <NA> C <NA>  
## 2722 1.0 62.19 <NA> N <NA>  
## 2723 1.0 63.09 <NA> C <NA>  
## 2724 1.0 68.70 <NA> C <NA>  
## 2725 1.0 69.17 <NA> O <NA>  
## 2726 1.0 55.41 <NA> C <NA>  
## 2727 1.0 57.25 <NA> C <NA>  
## 2728 1.0 60.34 <NA> C <NA>  
## 2729 1.0 75.53 <NA> N <NA>  
## 2730 1.0 83.10 <NA> C <NA>  
## 2731 1.0 84.21 <NA> C <NA>  
## 2732 1.0 82.93 <NA> O <NA>  
## 2733 1.0 89.71 <NA> C <NA>  
## 2734 1.0 93.81 <NA> C <NA>  
## 2735 1.0 97.60 <NA> C <NA>  
## 2736 1.0 94.39 <NA> C <NA>  
## 2737 1.0 96.09 <NA> N <NA>  
## 2738 1.0 88.40 <NA> N <NA>  
## 2739 1.0 92.48 <NA> C <NA>  
## 2740 1.0 90.47 <NA> C <NA>  
## 2741 1.0 89.39 <NA> O <NA>  
## 2742 1.0 98.20 <NA> C <NA>  
## 2743 1.0 99.61 <NA> C <NA>  
## 2744 1.0 94.89 <NA> C <NA>  
## 2745 1.0 88.64 <NA> N <NA>  
## 2746 1.0 85.75 <NA> C <NA>  
## 2747 1.0 80.52 <NA> C <NA>  
## 2748 1.0 78.32 <NA> O <NA>  
## 2749 1.0 89.63 <NA> C <NA>  
## 2750 1.0 99.02 <NA> C <NA>  
## 2751 1.0 102.07 <NA> C <NA>  
## 2752 1.0 103.98 <NA> O <NA>  
## 2753 1.0 104.35 <NA> O <NA>  
## 2754 1.0 78.09 <NA> N <NA>  
## 2755 1.0 68.95 <NA> C <NA>  
## 2756 1.0 62.92 <NA> C <NA>  
## 2757 1.0 62.03 <NA> O <NA>  
## 2758 1.0 62.36 <NA> N <NA>  
## 2759 1.0 58.58 <NA> C <NA>  
## 2760 1.0 54.84 <NA> C <NA>  
## 2761 1.0 50.93 <NA> O <NA>  
## 2762 1.0 60.08 <NA> C <NA>  
## 2763 1.0 61.50 <NA> C <NA>  
## 2764 1.0 56.60 <NA> C <NA>  
## 2765 1.0 54.23 <NA> C <NA>  
## 2766 1.0 63.55 <NA> N <NA>  
## 2767 1.0 55.13 <NA> N <NA>  
## 2768 1.0 58.10 <NA> C <NA>  
## 2769 1.0 58.32 <NA> C <NA>  
## 2770 1.0 60.62 <NA> O <NA>  
## 2771 1.0 55.63 <NA> C <NA>  
## 2772 1.0 56.25 <NA> C <NA>  
## 2773 1.0 52.59 <NA> O <NA>  
## 2774 1.0 53.79 <NA> O <NA>  
## 2775 1.0 59.46 <NA> N <NA>  
## 2776 1.0 59.79 <NA> C <NA>  
## 2777 1.0 62.04 <NA> C <NA>  
## 2778 1.0 61.87 <NA> O <NA>  
## 2779 1.0 53.91 <NA> C <NA>  
## 2780 1.0 47.41 <NA> C <NA>  
## 2781 1.0 56.61 <NA> O <NA>  
## 2782 1.0 46.22 <NA> O <NA>  
## 2783 1.0 67.19 <NA> N <NA>  
## 2784 1.0 71.10 <NA> C <NA>  
## 2785 1.0 70.62 <NA> C <NA>  
## 2786 1.0 75.90 <NA> O <NA>  
## 2787 1.0 71.67 <NA> C <NA>  
## 2788 1.0 75.99 <NA> C <NA>  
## 2789 1.0 67.52 <NA> C <NA>  
## 2790 1.0 69.66 <NA> N <NA>  
## 2791 1.0 73.02 <NA> C <NA>  
## 2792 1.0 76.86 <NA> C <NA>  
## 2793 1.0 74.63 <NA> O <NA>  
## 2794 1.0 67.49 <NA> C <NA>  
## 2795 1.0 61.94 <NA> O <NA>  
## 2796 1.0 63.16 <NA> C <NA>  
## 2797 1.0 80.11 <NA> N <NA>  
## 2798 1.0 84.85 <NA> C <NA>  
## 2799 1.0 87.94 <NA> C <NA>  
## 2800 1.0 92.68 <NA> O <NA>  
## 2801 1.0 90.50 <NA> N <NA>  
## 2802 1.0 91.56 <NA> C <NA>  
## 2803 1.0 93.10 <NA> C <NA>  
## 2804 1.0 92.89 <NA> O <NA>  
## 2805 1.0 89.34 <NA> C <NA>  
## 2806 1.0 89.69 <NA> C <NA>  
## 2807 1.0 90.04 <NA> C <NA>  
## 2808 1.0 93.88 <NA> O <NA>  
## 2809 1.0 89.58 <NA> O <NA>  
## 2810 1.0 94.43 <NA> N <NA>  
## 2811 1.0 93.14 <NA> C <NA>  
## 2812 1.0 90.52 <NA> C <NA>  
## 2813 1.0 90.17 <NA> O <NA>  
## 2814 1.0 98.13 <NA> C <NA>  
## 2815 1.0 107.66 <NA> C <NA>  
## 2816 1.0 114.09 <NA> C <NA>  
## 2817 1.0 114.94 <NA> O <NA>  
## 2818 1.0 119.84 <NA> O <NA>  
## 2819 1.0 87.62 <NA> N <NA>  
## 2820 1.0 84.68 <NA> C <NA>  
## 2821 1.0 88.42 <NA> C <NA>  
## 2822 1.0 88.22 <NA> O <NA>  
## 2823 1.0 74.14 <NA> C <NA>  
## 2824 1.0 65.86 <NA> C <NA>  
## 2825 1.0 67.02 <NA> C <NA>  
## 2826 1.0 61.86 <NA> C <NA>  
## 2827 1.0 92.78 <NA> N <NA>  
## 2828 1.0 90.46 <NA> C <NA>  
## 2829 1.0 89.00 <NA> C <NA>  
## 2830 1.0 88.20 <NA> O <NA>  
## 2831 1.0 90.31 <NA> C <NA>  
## 2832 1.0 89.90 <NA> O <NA>  
## 2833 1.0 95.72 <NA> C <NA>  
## 2834 1.0 83.39 <NA> N <NA>  
## 2835 1.0 78.00 <NA> C <NA>  
## 2836 1.0 73.58 <NA> C <NA>  
## 2837 1.0 73.09 <NA> O <NA>  
## 2838 1.0 77.13 <NA> C <NA>  
## 2839 1.0 85.41 <NA> O <NA>  
## 2840 1.0 76.17 <NA> C <NA>  
## 2841 1.0 69.35 <NA> N <NA>  
## 2842 1.0 64.70 <NA> C <NA>  
## 2843 1.0 66.24 <NA> C <NA>  
## 2844 1.0 62.29 <NA> O <NA>  
## 2845 1.0 56.35 <NA> C <NA>  
## 2846 1.0 67.98 <NA> C <NA>  
## 2847 1.0 75.18 <NA> C <NA>  
## 2848 1.0 79.21 <NA> N <NA>  
## 2849 1.0 80.17 <NA> C <NA>  
## 2850 1.0 82.43 <NA> N <NA>  
## 2851 1.0 85.42 <NA> N <NA>  
## 2852 1.0 73.28 <NA> N <NA>  
## 2853 1.0 76.27 <NA> C <NA>  
## 2854 1.0 73.63 <NA> C <NA>  
## 2855 1.0 71.12 <NA> O <NA>  
## 2856 1.0 83.68 <NA> C <NA>  
## 2857 1.0 94.60 <NA> C <NA>  
## 2858 1.0 102.79 <NA> C <NA>  
## 2859 1.0 105.31 <NA> C <NA>  
## 2860 1.0 108.27 <NA> N <NA>  
## 2861 1.0 74.18 <NA> N <NA>  
## 2862 1.0 72.06 <NA> C <NA>  
## 2863 1.0 66.36 <NA> C <NA>  
## 2864 1.0 67.51 <NA> O <NA>  
## 2865 1.0 83.65 <NA> C <NA>  
## 2866 1.0 95.07 <NA> C <NA>  
## 2867 1.0 94.29 <NA> O <NA>  
## 2868 1.0 105.04 <NA> O <NA>  
## 2869 1.0 56.14 <NA> N <NA>  
## 2870 1.0 48.30 <NA> C <NA>  
## 2871 1.0 45.46 <NA> C <NA>  
## 2872 1.0 49.01 <NA> O <NA>  
## 2873 1.0 48.61 <NA> C <NA>  
## 2874 1.0 48.99 <NA> C <NA>  
## 2875 1.0 54.01 <NA> O <NA>  
## 2876 1.0 55.57 <NA> O <NA>  
## 2877 1.0 45.41 <NA> N <NA>  
## 2878 1.0 49.98 <NA> C <NA>  
## 2879 1.0 43.67 <NA> C <NA>  
## 2880 1.0 51.86 <NA> O <NA>  
## 2881 1.0 54.98 <NA> C <NA>  
## 2882 1.0 65.69 <NA> C <NA>  
## 2883 1.0 75.73 <NA> C <NA>  
## 2884 1.0 79.12 <NA> O <NA>  
## 2885 1.0 84.62 <NA> N <NA>  
## 2886 1.0 41.24 <NA> N <NA>  
## 2887 1.0 41.98 <NA> C <NA>  
## 2888 1.0 40.19 <NA> C <NA>  
## 2889 1.0 45.73 <NA> O <NA>  
## 2890 1.0 46.38 <NA> C <NA>  
## 2891 1.0 43.30 <NA> C <NA>  
## 2892 1.0 42.65 <NA> C <NA>  
## 2893 1.0 47.97 <NA> O <NA>  
## 2894 1.0 57.57 <NA> O <NA>  
## 2895 1.0 45.06 <NA> N <NA>  
## 2896 1.0 51.63 <NA> C <NA>  
## 2897 1.0 49.54 <NA> C <NA>  
## 2898 1.0 51.31 <NA> O <NA>  
## 2899 1.0 62.15 <NA> C <NA>  
## 2900 1.0 78.37 <NA> C <NA>  
## 2901 1.0 85.82 <NA> C <NA>  
## 2902 1.0 88.86 <NA> O <NA>  
## 2903 1.0 88.83 <NA> O <NA>  
## 2904 1.0 44.46 <NA> N <NA>  
## 2905 1.0 38.98 <NA> C <NA>  
## 2906 1.0 38.03 <NA> C <NA>  
## 2907 1.0 37.72 <NA> O <NA>  
## 2908 1.0 48.24 <NA> C <NA>  
## 2909 1.0 59.62 <NA> O <NA>  
## 2910 1.0 46.18 <NA> C <NA>  
## 2911 1.0 35.32 <NA> N <NA>  
## 2912 1.0 25.16 <NA> C <NA>  
## 2913 1.0 28.19 <NA> C <NA>  
## 2914 1.0 36.62 <NA> O <NA>  
## 2915 1.0 20.40 <NA> C <NA>  
## 2916 1.0 4.81 <NA> C <NA>  
## 2917 1.0 19.93 <NA> C <NA>  
## 2918 1.0 29.57 <NA> N <NA>  
## 2919 1.0 25.74 <NA> C <NA>  
## 2920 1.0 25.80 <NA> C <NA>  
## 2921 1.0 35.56 <NA> O <NA>  
## 2922 1.0 28.50 <NA> C <NA>  
## 2923 1.0 30.35 <NA> C <NA>  
## 2924 1.0 31.72 <NA> C <NA>  
## 2925 1.0 39.92 <NA> N <NA>  
## 2926 1.0 37.41 <NA> C <NA>  
## 2927 1.0 45.07 <NA> N <NA>  
## 2928 1.0 32.76 <NA> N <NA>  
## 2929 1.0 29.71 <NA> N <NA>  
## 2930 1.0 34.69 <NA> C <NA>  
## 2931 1.0 34.15 <NA> C <NA>  
## 2932 1.0 41.71 <NA> O <NA>  
## 2933 1.0 40.87 <NA> C <NA>  
## 2934 1.0 55.98 <NA> C <NA>  
## 2935 1.0 69.72 <NA> C <NA>  
## 2936 1.0 77.72 <NA> C <NA>  
## 2937 1.0 82.99 <NA> N <NA>  
## 2938 1.0 32.99 <NA> N <NA>  
## 2939 1.0 31.89 <NA> C <NA>  
## 2940 1.0 34.22 <NA> C <NA>  
## 2941 1.0 35.85 <NA> O <NA>  
## 2942 1.0 25.71 <NA> C <NA>  
## 2943 1.0 28.41 <NA> C <NA>  
## 2944 0.5 30.64 <NA> C <NA>  
## 2945 0.5 29.76 <NA> N <NA>  
## 2946 0.5 32.13 <NA> C <NA>  
## 2947 0.5 30.84 <NA> N <NA>  
## 2948 0.5 27.72 <NA> N <NA>  
## 2949 1.0 30.78 <NA> N <NA>  
## 2950 1.0 27.26 <NA> C <NA>  
## 2951 1.0 27.72 <NA> C <NA>  
## 2952 1.0 32.62 <NA> O <NA>  
## 2953 1.0 23.82 <NA> C <NA>  
## 2954 1.0 30.70 <NA> C <NA>  
## 2955 1.0 28.31 <NA> C <NA>  
## 2956 1.0 20.56 <NA> C <NA>  
## 2957 1.0 28.78 <NA> N <NA>  
## 2958 1.0 32.04 <NA> C <NA>  
## 2959 1.0 29.24 <NA> C <NA>  
## 2960 1.0 35.28 <NA> O <NA>  
## 2961 1.0 36.27 <NA> C <NA>  
## 2962 1.0 41.31 <NA> C <NA>  
## 2963 1.0 39.56 <NA> C <NA>  
## 2964 1.0 27.31 <NA> N <NA>  
## 2965 1.0 30.02 <NA> C <NA>  
## 2966 1.0 29.20 <NA> C <NA>  
## 2967 1.0 34.79 <NA> O <NA>  
## 2968 1.0 39.60 <NA> C <NA>  
## 2969 1.0 61.97 <NA> C <NA>  
## 2970 1.0 74.59 <NA> C <NA>  
## 2971 1.0 76.47 <NA> O <NA>  
## 2972 1.0 79.94 <NA> O <NA>  
## 2973 1.0 27.40 <NA> N <NA>  
## 2974 1.0 22.24 <NA> C <NA>  
## 2975 1.0 26.18 <NA> C <NA>  
## 2976 1.0 30.38 <NA> O <NA>  
## 2977 1.0 24.65 <NA> C <NA>  
## 2978 1.0 24.88 <NA> C <NA>  
## 2979 1.0 19.94 <NA> C <NA>  
## 2980 1.0 17.20 <NA> C <NA>  
## 2981 1.0 14.35 <NA> C <NA>  
## 2982 1.0 17.48 <NA> C <NA>  
## 2983 1.0 18.36 <NA> C <NA>  
## 2984 1.0 27.55 <NA> O <NA>  
## 2985 1.0 27.05 <NA> N <NA>  
## 2986 1.0 29.56 <NA> C <NA>  
## 2987 1.0 29.86 <NA> C <NA>  
## 2988 1.0 36.73 <NA> O <NA>  
## 2989 1.0 27.82 <NA> C <NA>  
## 2990 1.0 27.65 <NA> C <NA>  
## 2991 1.0 31.11 <NA> N <NA>  
## 2992 1.0 23.13 <NA> C <NA>  
## 2993 1.0 36.57 <NA> C <NA>  
## 2994 1.0 31.35 <NA> N <NA>  
## 2995 1.0 30.06 <NA> N <NA>  
## 2996 1.0 36.78 <NA> C <NA>  
## 2997 1.0 35.66 <NA> C <NA>  
## 2998 1.0 36.00 <NA> O <NA>  
## 2999 1.0 43.46 <NA> C <NA>  
## 3000 1.0 60.67 <NA> C <NA>  
## 3001 1.0 75.54 <NA> C <NA>  
## 3002 1.0 79.95 <NA> O <NA>  
## 3003 1.0 78.32 <NA> N <NA>  
## 3004 1.0 37.48 <NA> N <NA>  
## 3005 1.0 35.24 <NA> C <NA>  
## 3006 1.0 33.47 <NA> C <NA>  
## 3007 1.0 38.42 <NA> O <NA>  
## 3008 1.0 41.55 <NA> C <NA>  
## 3009 1.0 42.48 <NA> C <NA>  
## 3010 1.0 62.60 <NA> S <NA>  
## 3011 1.0 46.90 <NA> C <NA>  
## 3012 1.0 27.53 <NA> N <NA>  
## 3013 1.0 25.10 <NA> C <NA>  
## 3014 1.0 28.43 <NA> C <NA>  
## 3015 1.0 30.30 <NA> O <NA>  
## 3016 1.0 23.22 <NA> C <NA>  
## 3017 1.0 26.83 <NA> O <NA>  
## 3018 1.0 27.97 <NA> C <NA>  
## 3019 1.0 25.89 <NA> N <NA>  
## 3020 1.0 20.81 <NA> C <NA>  
## 3021 1.0 15.73 <NA> C <NA>  
## 3022 1.0 20.68 <NA> O <NA>  
## 3023 1.0 25.39 <NA> C <NA>  
## 3024 1.0 14.03 <NA> N <NA>  
## 3025 1.0 15.32 <NA> C <NA>  
## 3026 1.0 20.84 <NA> C <NA>  
## 3027 1.0 23.30 <NA> O <NA>  
## 3028 1.0 12.31 <NA> C <NA>  
## 3029 1.0 10.00 <NA> C <NA>  
## 3030 1.0 13.00 <NA> C <NA>  
## 3031 1.0 23.29 <NA> N <NA>  
## 3032 1.0 22.38 <NA> C <NA>  
## 3033 1.0 19.71 <NA> C <NA>  
## 3034 1.0 22.87 <NA> O <NA>  
## 3035 1.0 24.08 <NA> C <NA>  
## 3036 1.0 23.51 <NA> C <NA>  
## 3037 1.0 27.12 <NA> C <NA>  
## 3038 1.0 7.32 <NA> C <NA>  
## 3039 1.0 24.37 <NA> N <NA>  
## 3040 1.0 16.24 <NA> C <NA>  
## 3041 1.0 17.05 <NA> C <NA>  
## 3042 1.0 21.78 <NA> O <NA>  
## 3043 1.0 22.39 <NA> C <NA>  
## 3044 1.0 24.54 <NA> C <NA>  
## 3045 1.0 18.51 <NA> C <NA>  
## 3046 1.0 32.49 <NA> C <NA>  
## 3047 1.0 15.27 <NA> N <NA>  
## 3048 1.0 8.75 <NA> C <NA>  
## 3049 1.0 8.75 <NA> C <NA>  
## 3050 1.0 13.07 <NA> O <NA>  
## 3051 1.0 16.58 <NA> N <NA>  
## 3052 1.0 17.70 <NA> C <NA>  
## 3053 1.0 19.92 <NA> C <NA>  
## 3054 1.0 24.93 <NA> O <NA>  
## 3055 1.0 14.78 <NA> C <NA>  
## 3056 1.0 23.20 <NA> C <NA>  
## 3057 1.0 22.58 <NA> C <NA>  
## 3058 1.0 24.76 <NA> C <NA>  
## 3059 1.0 15.70 <NA> C <NA>  
## 3060 1.0 31.29 <NA> C <NA>  
## 3061 1.0 22.52 <NA> C <NA>  
## 3062 1.0 32.12 <NA> O <NA>  
## 3063 1.0 19.08 <NA> N <NA>  
## 3064 1.0 15.15 <NA> C <NA>  
## 3065 1.0 18.36 <NA> C <NA>  
## 3066 1.0 31.46 <NA> O <NA>  
## 3067 1.0 12.85 <NA> C <NA>  
## 3068 1.0 8.71 <NA> C <NA>  
## 3069 1.0 18.08 <NA> C <NA>  
## 3070 1.0 7.44 <NA> C <NA>  
## 3071 1.0 5.86 <NA> C <NA>  
## 3072 1.0 10.64 <NA> C <NA>  
## 3073 1.0 14.36 <NA> C <NA>  
## 3074 1.0 20.64 <NA> O <NA>  
## 3075 1.0 20.91 <NA> N <NA>  
## 3076 1.0 22.04 <NA> C <NA>  
## 3077 1.0 18.20 <NA> C <NA>  
## 3078 1.0 24.53 <NA> O <NA>  
## 3079 1.0 21.39 <NA> C <NA>  
## 3080 1.0 38.19 <NA> O <NA>  
## 3081 1.0 17.98 <NA> N <NA>  
## 3082 1.0 22.57 <NA> C <NA>  
## 3083 1.0 20.33 <NA> C <NA>  
## 3084 1.0 24.19 <NA> O <NA>  
## 3085 1.0 31.27 <NA> C <NA>  
## 3086 1.0 37.02 <NA> C <NA>  
## 3087 1.0 52.37 <NA> C <NA>  
## 3088 1.0 57.09 <NA> C <NA>  
## 3089 1.0 54.13 <NA> N <NA>  
## 3090 1.0 18.89 <NA> N <NA>  
## 3091 1.0 17.40 <NA> C <NA>  
## 3092 1.0 18.81 <NA> C <NA>  
## 3093 1.0 21.73 <NA> O <NA>  
## 3094 1.0 12.07 <NA> C <NA>  
## 3095 1.0 21.07 <NA> C <NA>  
## 3096 1.0 31.67 <NA> C <NA>  
## 3097 1.0 31.48 <NA> O <NA>  
## 3098 1.0 38.11 <NA> O <NA>  
## 3099 1.0 18.16 <NA> N <NA>  
## 3100 1.0 16.89 <NA> C <NA>  
## 3101 1.0 24.93 <NA> C <NA>  
## 3102 1.0 28.97 <NA> O <NA>  
## 3103 1.0 18.94 <NA> C <NA>  
## 3104 1.0 31.76 <NA> N <NA>  
## 3105 1.0 32.72 <NA> C <NA>  
## 3106 1.0 30.67 <NA> C <NA>  
## 3107 1.0 36.59 <NA> O <NA>  
## 3108 1.0 44.24 <NA> C <NA>  
## 3109 1.0 62.20 <NA> C <NA>  
## 3110 1.0 73.36 <NA> C <NA>  
## 3111 1.0 74.91 <NA> O <NA>  
## 3112 1.0 78.46 <NA> O <NA>  
## 3113 1.0 29.99 <NA> N <NA>  
## 3114 1.0 27.62 <NA> C <NA>  
## 3115 1.0 30.46 <NA> C <NA>  
## 3116 1.0 37.39 <NA> O <NA>  
## 3117 1.0 33.19 <NA> C <NA>  
## 3118 1.0 35.86 <NA> N <NA>  
## 3119 1.0 28.81 <NA> C <NA>  
## 3120 1.0 29.18 <NA> C <NA>  
## 3121 1.0 34.90 <NA> O <NA>  
## 3122 1.0 31.05 <NA> N <NA>  
## 3123 1.0 30.80 <NA> C <NA>  
## 3124 1.0 30.51 <NA> C <NA>  
## 3125 1.0 31.26 <NA> O <NA>  
## 3126 1.0 35.28 <NA> C <NA>  
## 3127 1.0 37.72 <NA> C <NA>  
## 3128 1.0 45.12 <NA> O <NA>  
## 3129 1.0 39.51 <NA> N <NA>  
## 3130 1.0 28.17 <NA> N <NA>  
## 3131 1.0 26.13 <NA> C <NA>  
## 3132 1.0 26.64 <NA> C <NA>  
## 3133 1.0 30.09 <NA> O <NA>  
## 3134 1.0 24.83 <NA> C <NA>  
## 3135 1.0 21.97 <NA> O <NA>  
## 3136 1.0 25.37 <NA> C <NA>  
## 3137 1.0 26.92 <NA> N <NA>  
## 3138 1.0 24.41 <NA> C <NA>  
## 3139 1.0 18.31 <NA> C <NA>  
## 3140 1.0 23.38 <NA> O <NA>  
## 3141 1.0 26.07 <NA> C <NA>  
## 3142 1.0 36.62 <NA> C <NA>  
## 3143 1.0 61.81 <NA> C <NA>  
## 3144 1.0 67.59 <NA> C <NA>  
## 3145 1.0 63.20 <NA> N <NA>  
## 3146 1.0 25.04 <NA> N <NA>  
## 3147 1.0 14.69 <NA> C <NA>  
## 3148 1.0 21.73 <NA> C <NA>  
## 3149 1.0 22.36 <NA> O <NA>  
## 3150 1.0 14.99 <NA> C <NA>  
## 3151 1.0 13.65 <NA> C <NA>  
## 3152 1.0 17.01 <NA> C <NA>  
## 3153 1.0 19.51 <NA> C <NA>  
## 3154 1.0 18.87 <NA> C <NA>  
## 3155 1.0 16.69 <NA> C <NA>  
## 3156 1.0 19.64 <NA> C <NA>  
## 3157 1.0 24.53 <NA> O <NA>  
## 3158 1.0 22.44 <NA> N <NA>  
## 3159 1.0 16.48 <NA> C <NA>  
## 3160 1.0 18.64 <NA> C <NA>  
## 3161 1.0 21.76 <NA> O <NA>  
## 3162 1.0 22.94 <NA> C <NA>  
## 3163 1.0 28.81 <NA> N <NA>  
## 3164 1.0 30.51 <NA> C <NA>  
## 3165 1.0 31.72 <NA> C <NA>  
## 3166 1.0 37.20 <NA> O <NA>  
## 3167 1.0 34.07 <NA> C <NA>  
## 3168 1.0 36.49 <NA> C <NA>  
## 3169 1.0 49.99 <NA> C <NA>  
## 3170 1.0 61.44 <NA> C <NA>  
## 3171 1.0 64.95 <NA> N <NA>  
## 3172 1.0 27.06 <NA> N <NA>  
## 3173 1.0 21.88 <NA> C <NA>  
## 3174 1.0 22.72 <NA> C <NA>  
## 3175 1.0 27.11 <NA> O <NA>  
## 3176 1.0 17.90 <NA> C <NA>  
## 3177 1.0 19.19 <NA> C <NA>  
## 3178 1.0 21.51 <NA> C <NA>  
## 3179 1.0 28.75 <NA> N <NA>  
## 3180 1.0 25.29 <NA> C <NA>  
## 3181 1.0 24.93 <NA> C <NA>  
## 3182 1.0 27.95 <NA> O <NA>  
## 3183 1.0 27.71 <NA> C <NA>  
## 3184 1.0 26.58 <NA> C <NA>  
## 3185 1.0 26.21 <NA> O <NA>  
## 3186 1.0 42.69 <NA> O <NA>  
## 3187 1.0 23.56 <NA> N <NA>  
## 3188 1.0 23.39 <NA> C <NA>  
## 3189 1.0 28.12 <NA> C <NA>  
## 3190 1.0 33.42 <NA> O <NA>  
## 3191 1.0 34.03 <NA> N <NA>  
## 3192 1.0 34.89 <NA> C <NA>  
## 3193 1.0 33.45 <NA> C <NA>  
## 3194 1.0 43.30 <NA> O <NA>  
## 3195 1.0 25.77 <NA> C <NA>  
## 3196 1.0 28.87 <NA> O <NA>  
## 3197 1.0 25.19 <NA> C <NA>  
## 3198 1.0 31.82 <NA> N <NA>  
## 3199 1.0 28.10 <NA> C <NA>  
## 3200 1.0 32.66 <NA> C <NA>  
## 3201 1.0 32.43 <NA> O <NA>  
## 3202 1.0 16.90 <NA> C <NA>  
## 3203 1.0 19.85 <NA> C <NA>  
## 3204 1.0 20.39 <NA> C <NA>  
## 3205 1.0 21.38 <NA> C <NA>  
## 3206 1.0 32.66 <NA> N <NA>  
## 3207 1.0 40.73 <NA> N <NA>  
## 3208 1.0 41.23 <NA> C <NA>  
## 3209 1.0 36.11 <NA> C <NA>  
## 3210 1.0 33.86 <NA> O <NA>  
## 3211 1.0 45.50 <NA> C <NA>  
## 3212 1.0 42.55 <NA> C <NA>  
## 3213 1.0 37.11 <NA> C <NA>  
## 3214 1.0 33.77 <NA> N <NA>  
## 3215 1.0 34.49 <NA> C <NA>  
## 3216 1.0 31.45 <NA> C <NA>  
## 3217 1.0 39.11 <NA> O <NA>  
## 3218 1.0 33.02 <NA> C <NA>  
## 3219 1.0 41.67 <NA> C <NA>  
## 3220 1.0 37.01 <NA> C <NA>  
## 3221 1.0 31.49 <NA> N <NA>  
## 3222 1.0 23.62 <NA> C <NA>  
## 3223 1.0 24.28 <NA> C <NA>  
## 3224 1.0 23.82 <NA> O <NA>  
## 3225 1.0 35.36 <NA> C <NA>  
## 3226 1.0 28.04 <NA> N <NA>  
## 3227 1.0 28.03 <NA> C <NA>  
## 3228 1.0 29.07 <NA> C <NA>  
## 3229 1.0 30.28 <NA> O <NA>  
## 3230 1.0 31.68 <NA> C <NA>  
## 3231 1.0 31.63 <NA> C <NA>  
## 3232 1.0 51.58 <NA> C <NA>  
## 3233 1.0 49.89 <NA> O <NA>  
## 3234 1.0 61.19 <NA> O <NA>  
## 3235 1.0 28.11 <NA> N <NA>  
## 3236 1.0 26.22 <NA> C <NA>  
## 3237 1.0 23.94 <NA> C <NA>  
## 3238 1.0 29.50 <NA> O <NA>  
## 3239 1.0 33.28 <NA> C <NA>  
## 3240 1.0 27.17 <NA> C <NA>  
## 3241 1.0 25.81 <NA> C <NA>  
## 3242 1.0 21.18 <NA> N <NA>  
## 3243 1.0 23.40 <NA> C <NA>  
## 3244 1.0 27.50 <NA> C <NA>  
## 3245 1.0 31.74 <NA> O <NA>  
## 3246 1.0 14.01 <NA> C <NA>  
## 3247 1.0 31.33 <NA> C <NA>  
## 3248 1.0 47.99 <NA> C <NA>  
## 3249 1.0 64.20 <NA> N <NA>  
## 3250 1.0 74.24 <NA> C <NA>  
## 3251 1.0 78.57 <NA> N <NA>  
## 3252 1.0 79.06 <NA> N <NA>  
## 3253 1.0 29.51 <NA> N <NA>  
## 3254 1.0 21.31 <NA> C <NA>  
## 3255 1.0 30.49 <NA> C <NA>  
## 3256 1.0 31.94 <NA> O <NA>  
## 3257 1.0 27.53 <NA> C <NA>  
## 3258 1.0 30.32 <NA> N <NA>  
## 3259 1.0 29.85 <NA> C <NA>  
## 3260 1.0 30.05 <NA> C <NA>  
## 3261 1.0 27.04 <NA> O <NA>  
## 3262 1.0 31.66 <NA> C <NA>  
## 3263 1.0 38.57 <NA> C <NA>  
## 3264 1.0 42.73 <NA> O <NA>  
## 3265 1.0 38.85 <NA> O <NA>  
## 3266 1.0 23.62 <NA> N <NA>  
## 3267 1.0 18.00 <NA> C <NA>  
## 3268 1.0 23.95 <NA> C <NA>  
## 3269 1.0 29.62 <NA> O <NA>  
## 3270 1.0 13.98 <NA> C <NA>  
## 3271 1.0 20.60 <NA> C <NA>  
## 3272 1.0 17.69 <NA> C <NA>  
## 3273 1.0 17.56 <NA> C <NA>  
## 3274 1.0 29.96 <NA> N <NA>  
## 3275 1.0 34.24 <NA> C <NA>  
## 3276 1.0 35.97 <NA> C <NA>  
## 3277 1.0 39.44 <NA> O <NA>  
## 3278 1.0 36.22 <NA> C <NA>  
## 3279 1.0 50.16 <NA> C <NA>  
## 3280 1.0 58.26 <NA> C <NA>  
## 3281 1.0 60.21 <NA> O <NA>  
## 3282 1.0 62.44 <NA> O <NA>  
## 3283 1.0 39.54 <NA> N <NA>  
## 3284 1.0 45.82 <NA> C <NA>  
## 3285 1.0 45.32 <NA> C <NA>  
## 3286 1.0 41.65 <NA> O <NA>  
## 3287 1.0 56.42 <NA> C <NA>  
## 3288 1.0 65.10 <NA> C <NA>  
## 3289 1.0 73.03 <NA> C <NA>  
## 3290 1.0 76.00 <NA> C <NA>  
## 3291 1.0 70.33 <NA> N <NA>  
## 3292 1.0 43.16 <NA> N <NA>  
## 3293 1.0 42.82 <NA> C <NA>  
## 3294 1.0 40.58 <NA> C <NA>  
## 3295 1.0 40.69 <NA> O <NA>  
## 3296 1.0 39.87 <NA> C <NA>  
## 3297 1.0 32.71 <NA> C <NA>  
## 3298 1.0 43.73 <NA> C <NA>  
## 3299 1.0 35.56 <NA> C <NA>  
## 3300 1.0 38.78 <NA> N <NA>  
## 3301 1.0 39.78 <NA> C <NA>  
## 3302 1.0 47.57 <NA> C <NA>  
## 3303 1.0 55.44 <NA> O <NA>  
## 3304 1.0 32.19 <NA> C <NA>  
## 3305 1.0 26.04 <NA> C <NA>  
## 3306 1.0 29.00 <NA> C <NA>  
## 3307 1.0 24.49 <NA> C <NA>  
## 3308 1.0 54.94 <NA> N <NA>  
## 3309 1.0 61.27 <NA> C <NA>  
## 3310 1.0 69.53 <NA> C <NA>  
## 3311 1.0 78.47 <NA> O <NA>  
## 3312 1.0 71.89 <NA> O <NA>  
## 3313 1.0 28.52 <NA> O <NA>  
## 3314 1.0 55.00 <NA> O <NA>  
## 3315 1.0 31.07 <NA> O <NA>  
## 3316 1.0 39.91 <NA> O <NA>  
## 3317 1.0 29.11 <NA> O <NA>  
## 3318 1.0 23.58 <NA> O <NA>  
## 3319 1.0 24.48 <NA> O <NA>  
## 3320 1.0 30.73 <NA> O <NA>  
## 3321 1.0 29.89 <NA> O <NA>  
## 3322 1.0 34.71 <NA> O <NA>  
## 3323 1.0 29.39 <NA> O <NA>  
## 3324 1.0 18.63 <NA> O <NA>  
## 3325 1.0 33.11 <NA> O <NA>  
## 3326 1.0 41.02 <NA> O <NA>  
## 3327 1.0 39.60 <NA> O <NA>  
## 3328 1.0 34.63 <NA> O <NA>  
## 3329 1.0 37.43 <NA> O <NA>  
## 3330 1.0 44.62 <NA> O <NA>  
## 3331 1.0 39.14 <NA> O <NA>  
## 3332 1.0 36.12 <NA> O <NA>  
## 3333 1.0 40.37 <NA> O <NA>  
## 3334 1.0 76.22 <NA> O <NA>  
## 3335 1.0 64.47 <NA> O <NA>  
## 3336 1.0 42.83 <NA> O <NA>  
## 3337 1.0 51.42 <NA> O <NA>  
## 3338 1.0 47.03 <NA> O <NA>  
## 3339 1.0 47.59 <NA> O <NA>  
## 3340 1.0 40.93 <NA> O <NA>  
## 3341 1.0 30.58 <NA> O <NA>  
## 3342 1.0 48.61 <NA> O <NA>  
## 3343 1.0 61.76 <NA> O <NA>  
## 3344 1.0 75.55 <NA> O <NA>  
## 3345 1.0 43.78 <NA> O <NA>  
## 3346 1.0 25.32 <NA> O <NA>  
## 3347 1.0 26.42 <NA> O <NA>  
## 3348 1.0 35.75 <NA> O <NA>  
## 3349 1.0 36.17 <NA> O <NA>  
## 3350 1.0 40.76 <NA> O <NA>  
## 3351 1.0 38.38 <NA> O <NA>  
## 3352 1.0 37.15 <NA> O <NA>  
## 3353 1.0 52.72 <NA> O <NA>  
## 3354 1.0 56.12 <NA> O <NA>  
## 3355 1.0 50.34 <NA> O <NA>  
## 3356 1.0 40.13 <NA> O <NA>  
## 3357 1.0 47.15 <NA> O <NA>  
## 3358 1.0 33.77 <NA> O <NA>  
## 3359 1.0 76.43 <NA> O <NA>  
## 3360 1.0 34.50 <NA> O <NA>  
## 3361 1.0 63.43 <NA> O <NA>  
## 3362 1.0 91.26 <NA> O <NA>  
## 3363 1.0 73.81 <NA> O <NA>  
## 3364 1.0 45.51 <NA> O <NA>  
## 3365 1.0 61.63 <NA> O <NA>  
## 3366 1.0 68.03 <NA> O <NA>  
## 3367 1.0 72.53 <NA> O <NA>  
## 3368 1.0 68.16 <NA> O <NA>  
## 3369 1.0 60.11 <NA> O <NA>  
## 3370 1.0 71.80 <NA> O <NA>  
## 3371 1.0 49.64 <NA> O <NA>  
## 3372 1.0 58.23 <NA> O <NA>  
## 3373 1.0 45.67 <NA> O <NA>  
## 3374 1.0 64.70 <NA> O <NA>  
## 3375 1.0 93.29 <NA> O <NA>  
## 3376 1.0 81.88 <NA> O <NA>  
## 3377 1.0 63.37 <NA> O <NA>  
## 3378 1.0 59.95 <NA> O <NA>  
## 3379 1.0 41.18 <NA> O <NA>  
## 3380 1.0 55.10 <NA> O <NA>  
## 3381 1.0 56.01 <NA> O <NA>  
## 3382 1.0 60.69 <NA> O <NA>  
## 3383 1.0 74.05 <NA> O <NA>  
## 3384 1.0 83.13 <NA> O <NA>  
## 3385 1.0 21.95 <NA> O <NA>  
## 3386 1.0 32.61 <NA> O <NA>  
## 3387 1.0 28.57 <NA> O <NA>  
## 3388 1.0 30.22 <NA> O <NA>  
## 3389 1.0 34.86 <NA> O <NA>  
## 3390 1.0 34.06 <NA> O <NA>  
## 3391 1.0 36.22 <NA> O <NA>  
## 3392 1.0 37.07 <NA> O <NA>  
## 3393 1.0 27.21 <NA> O <NA>  
## 3394 1.0 27.63 <NA> O <NA>  
## 3395 1.0 50.16 <NA> O <NA>  
## 3396 1.0 40.20 <NA> O <NA>  
## 3397 1.0 27.58 <NA> O <NA>  
## 3398 1.0 30.28 <NA> O <NA>  
## 3399 1.0 40.43 <NA> O <NA>  
## 3400 1.0 39.49 <NA> O <NA>  
## 3401 1.0 46.46 <NA> O <NA>  
## 3402 1.0 34.28 <NA> O <NA>  
## 3403 1.0 32.99 <NA> O <NA>  
## 3404 1.0 34.51 <NA> O <NA>  
## 3405 1.0 42.61 <NA> O <NA>  
## 3406 1.0 43.59 <NA> O <NA>  
## 3407 1.0 34.54 <NA> O <NA>  
## 3408 1.0 41.07 <NA> O <NA>  
## 3409 1.0 50.54 <NA> O <NA>  
## 3410 1.0 38.94 <NA> O <NA>  
## 3411 1.0 42.04 <NA> O <NA>  
## 3412 1.0 50.01 <NA> O <NA>  
## 3413 1.0 43.99 <NA> O <NA>  
## 3414 1.0 35.30 <NA> O <NA>  
## 3415 1.0 50.08 <NA> O <NA>  
## 3416 1.0 44.38 <NA> O <NA>  
## 3417 1.0 38.22 <NA> O <NA>  
## 3418 1.0 34.89 <NA> O <NA>  
## 3419 1.0 49.56 <NA> O <NA>  
## 3420 1.0 51.45 <NA> O <NA>  
## 3421 1.0 45.41 <NA> O <NA>  
## 3422 1.0 59.89 <NA> O <NA>  
## 3423 1.0 65.53 <NA> O <NA>  
## 3424 1.0 51.04 <NA> O <NA>  
## 3425 1.0 54.31 <NA> O <NA>  
## 3426 1.0 48.91 <NA> O <NA>  
## 3427 1.0 51.89 <NA> O <NA>  
## 3428 1.0 51.54 <NA> O <NA>  
## 3429 1.0 51.29 <NA> O <NA>  
## 3430 1.0 55.89 <NA> O <NA>  
## 3431 1.0 64.21 <NA> O <NA>  
## 3432 1.0 56.73 <NA> O <NA>  
## 3433 1.0 76.38 <NA> O <NA>  
## 3434 1.0 53.42 <NA> O <NA>  
## 3435 1.0 48.15 <NA> O <NA>  
## 3436 1.0 57.10 <NA> O <NA>  
## 3437 1.0 47.62 <NA> O <NA>  
## 3438 1.0 71.54 <NA> O <NA>  
## 3439 1.0 89.95 <NA> O <NA>  
## 3440 1.0 53.67 <NA> O <NA>  
## 3441 1.0 58.97 <NA> O <NA>  
## 3442 1.0 49.96 <NA> O <NA>  
## 3443 1.0 65.65 <NA> O <NA>  
## 3444 1.0 58.74 <NA> O <NA>  
## 3445 1.0 59.83 <NA> O <NA>  
## 3446 1.0 63.80 <NA> O <NA>  
## 3447 1.0 70.36 <NA> O <NA>  
## 3448 1.0 55.70 <NA> O <NA>  
## 3449 1.0 65.19 <NA> O <NA>  
## 3450 1.0 57.23 <NA> O <NA>  
## 3451 1.0 53.76 <NA> O <NA>  
## 3452 1.0 42.85 <NA> O <NA>  
## 3453 1.0 44.15 <NA> O <NA>  
## 3454 1.0 52.01 <NA> O <NA>  
## 3455 1.0 81.32 <NA> O <NA>  
## 3456 1.0 77.22 <NA> O <NA>  
## 3457 1.0 42.17 <NA> O <NA>  
## 3458 1.0 86.54 <NA> O <NA>  
## 3459 1.0 69.58 <NA> O <NA>

plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")  
points(s2.b, typ = "l", col = "blue", lwd= 1)  
points(s3.b, typ = "l", col = "red", lwd = 1)



hc <- hclust( dist( rbind(s1.b, s2.b, s3.b) ) )  
plot(hc)



Q1. What type of object is returned from the read.pdb() function? **returns a large list from protein database. Can tell it is a list by using str() function on s1, s2, or s3. It is a list of 8 things and of class “pdb”**

Q2. What does the trim.pdb() function do? **Produces a new smaller PDB object, containing a subset of atoms, from a given larger PDB object**

Q3. What input parameter would turn off the marginal black and grey rectangles in the plots and what do they represent in this case? **You can remove the elety=“CA” to remove the black and grey rectangles. They represent a character vector of atom names**

Q4. What would be a better plot to compare across the different proteins? **overlay the graphs using points()**

Q5. Which proteins are more similar to each other in their B-factor trends. How could you quantify this? HINT: try the rbind(), dist() and hclust() functions together with a resulting dendrogram plot. Look up the documentation to see what each of these functions does. **s2 and s3 are closer to each other according to hclust(), rbind(), dist() function**

Q6. How would you generalize the original code above to work with any set of input protein structures?