Class 6: R Function

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# Functions

Read table functions 1. read.table(“filename.txt”, header=TRUE, sep=")

1. separater type consists of ," is comma, “;” is semicolin, "" is white space
2. read.delim

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", header=TRUE, sep=",")  
t1

## Col1 Col2 Col3  
## 1 1 2 3  
## 2 4 5 6  
## 3 7 8 9  
## 4 a b c

You could also use read.csv which has the arguments I want in this case.

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

## Col1 Col2 Col3  
## 1 1 2 3  
## 2 4 5 6  
## 3 7 8 9  
## 4 a b c

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

## Col1 Col2 Col3  
## 1 1 2 3  
## 2 4 5 6  
## 3 7 8 9  
## 4 a b c

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

## V1 V2 V3  
## 1 1 6 a  
## 2 2 7 b  
## 3 3 8 c  
## 4 4 9 d  
## 5 5 10 e

# Back To Functions

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

using this function

add(7,3)

## [1] 10

add(x=1, y=4)

## [1] 5

add(1, 4)

## [1] 5

add(1)

## [1] 2

add(3)

## [1] 4

How does this work with ventors?

add( c(1, 2, 4) )

## [1] 2 3 5

add( c(1, 2, 4), 4 )

## [1] 5 6 8

add( c(1, 2, 4), c(4, 5, 6) )

## [1] 5 7 10

What is this range() function?

x <- c(4,4,10,11,1)  
max(x)

## [1] 11

min (x)

## [1] 1

range(x)

## [1] 1 11

rng <- range(x)  
rng

## [1] 1 11

This is our second function

rescale <- function(x) {  
 rng <-range(x)  
 (x - rng[1]) / (rng[2] - rng[1])  
}  
rescale(1:10)

## [1] 0.0000000 0.1111111 0.2222222 0.3333333 0.4444444 0.5555556 0.6666667  
## [8] 0.7777778 0.8888889 1.0000000

rescale( c(1,2,NA,3,10) )

## [1] NA NA NA NA NA

rescale2 <- function(x) {  
 rng <- range (x, na.rm=TRUE)  
 (x - rng[1]) / (rng[2] - rng[1])  
}

rescale2( c(1,2,NA,3,10) )

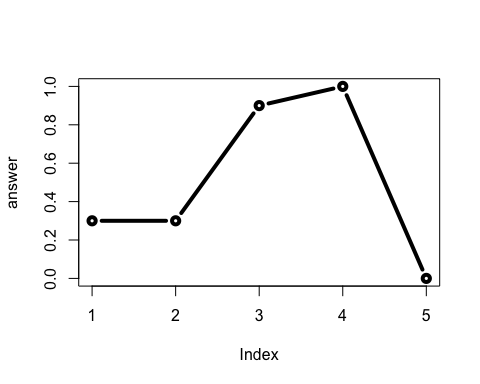
## [1] 0.0000000 0.1111111 NA 0.2222222 1.0000000

Going too far!

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) {  
 print("don't sing again")  
 plot(answer, typ="b", lwd=4)  
 }  
 print("I can see it in ...")  
 return(answer)  
}

rescale3(x, plot=TRUE)

## [1] "Hello"  
## [1] "is it me you are looking for?"  
## [1] "don't sing again"



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

## [1] 0.3 0.3 0.9 1.0 0.0

rescale3(x, plot=FALSE)

## [1] "Hello"  
## [1] "is it me you are looking for?"  
## [1] "I can see it in ..."

## [1] 0.3 0.3 0.9 1.0 0.0

## Hands on Worksheet Part B

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

## Note: Accessing on-line PDB file

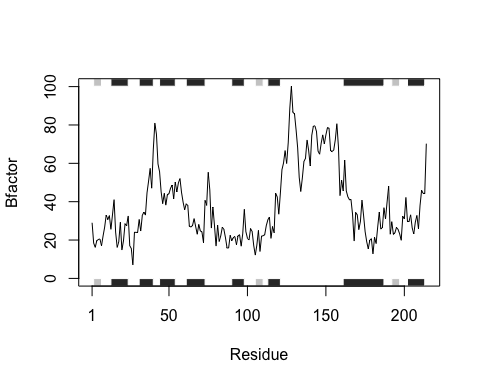
s2 <- read.pdb("1AKE") # kinase no drug

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

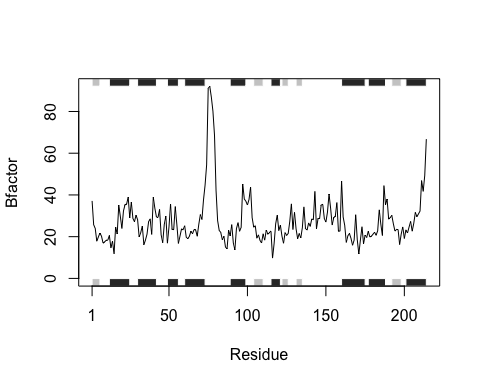
s3 <- read.pdb("1E4Y") # kinase with drug

## Note: Accessing on-line PDB file

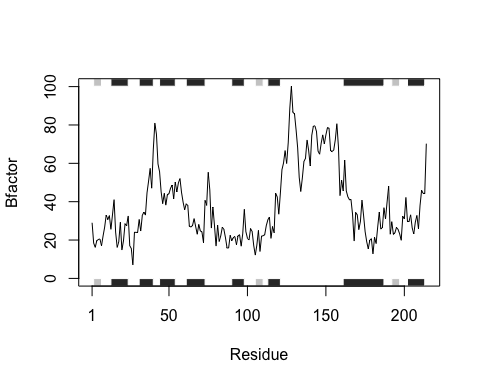
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")  
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")  
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")  
  
s1.b <- s1.chainA$atom$b  
s2.b <- s2.chainA$atom$b  
s3.b <- s3.chainA$atom$b  
  
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")



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



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

 Q1. What type of object is returned from the read.pdb() function? It is a list of 8 things and of class “pdb”, “sse”

s1

##   
## Call: read.pdb(file = "4AKE")  
##   
## Total Models#: 1  
## Total Atoms#: 3459, XYZs#: 10377 Chains#: 2 (values: A B)  
##   
## Protein Atoms#: 3312 (residues/Calpha atoms#: 428)  
## Nucleic acid Atoms#: 0 (residues/phosphate atoms#: 0)  
##   
## Non-protein/nucleic Atoms#: 147 (residues: 147)  
## Non-protein/nucleic resid values: [ HOH (147) ]  
##   
## Protein sequence:  
## MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAAVKSGSELGKQAKDIMDAGKLVT  
## DELVIALVKERIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVDRI  
## VGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKDDQEETVRKRLVEYHQMTAPLIG  
## YYSKEAEAGNTKYAKVDGTKPVAEVRADLEKILGMRIILLGAPGA...<cut>...KILG  
##   
## + attr: atom, xyz, seqres, helix, sheet,  
## calpha, remark, call

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"

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  
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## 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  
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## 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  
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## 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  
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## 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  
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## 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  
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## 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  
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## 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  
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## 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  
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## 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  
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## 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  
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## 1045 ATOM 1045 CG <NA> PHE A 137 <NA> -4.126 1.228 -31.557  
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## 1049 ATOM 1049 CE2 <NA> PHE A 137 <NA> -2.128 0.640 -30.327  
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## 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  
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## 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  
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## 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  
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## 1065 ATOM 1065 CD <NA> PRO A 139 <NA> -7.448 6.604 -34.570  
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## 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  
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## 1072 ATOM 1072 CD <NA> PRO A 140 <NA> -7.352 11.488 -32.142  
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## 1074 ATOM 1074 CA <NA> LYS A 141 <NA> -11.703 12.964 -35.707  
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## 1079 ATOM 1079 CD <NA> LYS A 141 <NA> -15.564 12.893 -35.191  
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## 1081 ATOM 1081 NZ <NA> LYS A 141 <NA> -17.664 12.574 -33.885  
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## 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  
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## 1087 ATOM 1087 CG1 <NA> VAL A 142 <NA> -9.603 18.746 -35.315  
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## 1090 ATOM 1090 CA <NA> GLU A 143 <NA> -6.442 14.821 -34.608  
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## 1099 ATOM 1099 CA <NA> GLY A 144 <NA> -5.069 16.360 -31.402  
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## 1101 ATOM 1101 O <NA> GLY A 144 <NA> -5.901 17.828 -29.699  
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## 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  
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## 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  
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## 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  
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## 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  
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## 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  
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## 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  
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## 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  
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## 1683 ATOM 1684 CD1 <NA> ILE B 3 <NA> -9.119 22.014 14.806  
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## 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  
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## 1697 ATOM 1698 CG <NA> LEU B 5 <NA> -5.168 15.012 16.636  
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## 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  
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## 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  
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## 1716 ATOM 1717 CB <NA> ALA B 8 <NA> 3.093 8.412 20.193  
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## 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  
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## 1727 ATOM 1728 O <NA> GLY B 10 <NA> -1.585 5.332 23.239  
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## 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  
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## 1738 ATOM 1739 CA <NA> LYS B 13 <NA> -5.471 11.450 20.366  
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## 1741 ATOM 1742 CB <NA> LYS B 13 <NA> -4.507 11.961 19.289  
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## 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  
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## 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  
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## 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  
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## 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  
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## 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  
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## 1796 ATOM 1797 CG1 <NA> ILE B 20 <NA> -10.906 18.699 18.486  
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## 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  
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## 1815 ATOM 1816 OE2 <NA> GLU B 22 <NA> -21.988 17.226 20.530  
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## 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  
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## 1821 ATOM 1822 CG <NA> LYS B 23 <NA> -15.797 23.691 19.527  
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## 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  
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## 1830 ATOM 1831 CG <NA> TYR B 24 <NA> -14.074 23.839 15.704  
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## 1840 ATOM 1841 O <NA> GLY B 25 <NA> -17.829 21.564 10.062  
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## 1847 ATOM 1848 CG2 <NA> ILE B 26 <NA> -14.484 22.046 10.837  
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## 1858 ATOM 1859 C <NA> GLN B 28 <NA> -11.477 13.306 9.078  
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## 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  
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## 1866 ATOM 1867 CA <NA> ILE B 29 <NA> -9.644 13.060 7.508  
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## 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  
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## 1881 ATOM 1882 C <NA> THR B 31 <NA> -5.409 8.072 3.943  
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## 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  
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## 1891 ATOM 1892 CA <NA> ASP B 33 <NA> -9.514 6.261 4.370  
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## 1894 ATOM 1895 CB <NA> ASP B 33 <NA> -10.440 7.083 5.286  
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## 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  
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## 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  
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## 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  
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## 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  
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## 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  
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## 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  
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## 2357 ATOM 2358 CB <NA> ASP B 94 <NA> 7.750 21.007 2.111  
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## 2359 ATOM 2360 OD1 <NA> ASP B 94 <NA> 8.258 23.321 1.959  
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## 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  
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## 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  
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## 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  
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## 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  
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## 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  
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## 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  
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## 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  
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## 3050 ATOM 3051 O <NA> GLY B 180 <NA> 10.285 23.345 13.714  
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## 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  
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## 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  
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## 3080 ATOM 3081 OG <NA> SER B 183 <NA> 7.913 23.226 17.331  
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## 3089 ATOM 3090 NZ <NA> LYS B 184 <NA> 15.514 26.360 12.611  
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## 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  
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## 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  
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## 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  
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## 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  
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## 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  
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## 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  
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## 3133 ATOM 3134 O <NA> THR B 191 <NA> 1.345 29.390 13.752  
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## 3136 ATOM 3137 CG2 <NA> THR B 191 <NA> 1.834 26.458 11.875  
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## 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  
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## 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  
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## 3157 ATOM 3158 OH <NA> TYR B 193 <NA> 4.826 20.099 19.571  
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## 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  
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## 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  
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## 3206 ATOM 3207 NZ <NA> LYS B 200 <NA> -3.163 20.545 31.604  
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## 3208 ATOM 3209 CA <NA> PRO B 201 <NA> -8.222 13.333 32.534  
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## 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  
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## 3220 ATOM 3221 CG2 <NA> VAL B 202 <NA> -10.418 11.269 28.508  
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## 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  
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## 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>

Q2. What does the trim.pdb() function do?

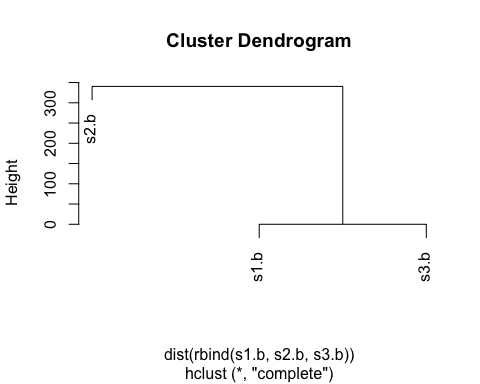
It makes it smaller.

Q3. What input parameter would turn off the marginal black and grey rectangles in the  
plots and what do they represent in this case?  
  
  
Q4. What would be a better plot to compare across the different proteins?  
If the 3 plots where put together into 1 plot.

```

Q5. Which proteins are more similar to each other in their B-factor trends. How could you quantify this? s1.b and s3.b are more similar to each other

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



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

### Level 3 Heading