

fig5_v2

2025-06-13

```
## Loading required package: digest

## Loading required package: tibble

## Loading required package: ggplot2

## Project name: 01.protein-seq-evo-v1

## Loading project configuration

## Autoloading packages

## Loading package: dplyr

## Loading required package: dplyr

##
## Attaching package: 'dplyr'

## The following objects are masked from 'package:stats':
##
##   filter, lag

## The following objects are masked from 'package:base':
##
##   intersect, setdiff, setequal, union

## Loading package: stringr

## Loading required package: stringr

## Loading package: readr

## Loading required package: readr

## Loading package: ggplot2

## Loading package: tidyr

## Loading required package: tidyr
```

```

## Loading package: patchwork

## Loading required package: patchwork

## Loading package: gridExtra

## Loading required package: gridExtra

##
## Attaching package: 'gridExtra'

## The following object is masked from 'package:dplyr':
##
##   combine

## Loading package: GGally

## Loading required package: GGally

## Registered S3 method overwritten by 'GGally':
##   method from
##   +.gg      ggplot2

## Loading package: readxl

## Loading required package: readxl

## Loading package: viridis

## Loading required package: viridis

## Loading required package: viridisLite

## Loading package: cowplot

## Loading required package: cowplot

##
## Attaching package: 'cowplot'

## The following object is masked from 'package:patchwork':
##
##   align_plots

## Loading package: ggsignif

## Loading required package: ggsignif

## Loading package: minpack.lm

```

```

## Loading required package: minpack.lm

## Loading package: purrr

## Loading required package: purrr

## Loading package: scales

## Loading required package: scales

##
## Attaching package: 'scales'

## The following object is masked from 'package:purrr':
##
##     discard

## The following object is masked from 'package:viridis':
##
##     viridis_pal

## The following object is masked from 'package:readr':
##
##     col_factor

## Loading package: bigsnpr

## Loading required package: bigsnpr

## Loading required package: bigstatsr

## Loading package: drc

## Loading required package: drc

## Loading required package: MASS

##
## Attaching package: 'MASS'

## The following object is masked from 'package:patchwork':
##
##     area

## The following object is masked from 'package:dplyr':
##
##     select

##
## 'drc' has been loaded.

```

```

## Please cite R and 'drc' if used for a publication,

## for references type 'citation()' and 'citation('drc')'.

##
## Attaching package: 'drc'

## The following objects are masked from 'package:stats':
##
##     gaussian, getInitial

## Loading package: data.table

## Loading required package: data.table

##
## Attaching package: 'data.table'

## The following object is masked from 'package:purrr':
##
##     transpose

## The following objects are masked from 'package:dplyr':
##
##     between, first, last

## Autoloading helper functions

## Running helper script: globals.R

## Running helper script: helpers.R

## Autoloading data

## Munging data

## Running preprocessing script: 01-util.R

## Sourcing R script: 01-util.R

## Running preprocessing script: 02-munge_kras.R

## Sourcing R script: 02-munge_kras.R

## Rows: 189 Columns: 8
## -- Column specification -----
## Delimiter: "\t"
## chr (6): SEQ, ATOM, COLOR, CONFIDENCE INTERVAL, MSA DATA, RESIDUE VARIETY
## dbl (2): POS, SCORE

```

```

##
## i Use 'spec()' to retrieve the full column specification for this data.
## i Specify the column types or set 'show_col_types = FALSE' to quiet this message.
## Rows: 3591 Columns: 4
## -- Column specification -----
## Delimiter: "\t"
## chr (3): X1, X2, X4
## dbl (1): X3
##
## i Use 'spec()' to retrieve the full column specification for this data.
## i Specify the column types or set 'show_col_types = FALSE' to quiet this message.
## Rows: 3780 Columns: 3
## -- Column specification -----
## Delimiter: ","
## chr (1): variant
## dbl (2): score, pos
##
## i Use 'spec()' to retrieve the full column specification for this data.
## i Specify the column types or set 'show_col_types = FALSE' to quiet this message.
## Rows: 3572 Columns: 15
## -- Column specification -----
## Delimiter: ","
## chr (1): mutant
## dbl (11): column_coverage, popEVE, pop-adjusted_ESM1v, pop-adjusted_EVH_epis...
## lgl (3): pop-adjusted_EVE, pop-adjusted_Tranception, EVE
##
## i Use 'spec()' to retrieve the full column specification for this data.
## i Specify the column types or set 'show_col_types = FALSE' to quiet this message.
## Rows: 3780 Columns: 43
## -- Column specification -----
## Delimiter: ","
## chr (18): wt_aa, mt_aa, ClinVar_ClinicalSignificance, Starred_Coarse_Grained...
## dbl (11): position, Gold_Stars, NumberSubmitters, frequency_gv2, frequency_g...
## lgl (14): BS1, PM2, PM5, PP5, BP6, b_model, p_model, b_acmg_model, lb_acmg_m...
##
## i Use 'spec()' to retrieve the full column specification for this data.
## i Specify the column types or set 'show_col_types = FALSE' to quiet this message.
## Rows: 2587 Columns: 28
## -- Column specification -----
## Delimiter: ","
## chr (8): id, wt_aa, mt_aa, bp_interface, binding_RAF, binding_RAL, binding...
## dbl (20): Pos_real, abundance_ddg, abundance_ddg_std, pik3cg_ddg, pik3cg_ddg...
##
## i Use 'spec()' to retrieve the full column specification for this data.
## i Specify the column types or set 'show_col_types = FALSE' to quiet this message.
## Rows: 3453 Columns: 6
## -- Column specification -----
## Delimiter: ","
## chr (2): id, wt_codon
## dbl (4): Pos_real, mean_kcal/mol, std_kcal/mol, ESM1v
##
## i Use 'spec()' to retrieve the full column specification for this data.
## i Specify the column types or set 'show_col_types = FALSE' to quiet this message.
## Running preprocessing script: 03-munge_src.R

```

```

##
## Sourcing R script: 03-munge_src.R
##
## Rows: 5112 Columns: 9
## -- Column specification -----
## Delimiter: " "
## chr (1): id
## dbl (8): FL_activity_mean_kcal/mol, FL_activity_std_kcal/mol, FL_folding_mea...
##
## i Use 'spec()' to retrieve the full column specification for this data.
## i Specify the column types or set 'show_col_types = FALSE' to quiet this message.
## Rows: 536 Columns: 8
## -- Column specification -----
## Delimiter: "\t"
## chr (6): SEQ, ATOM, COLOR, CONFIDENCE INTERVAL, MSA DATA, RESIDUE VARIETY
## dbl (2): POS, SCORE
##
## i Use 'spec()' to retrieve the full column specification for this data.
## i Specify the column types or set 'show_col_types = FALSE' to quiet this message.
## Rows: 10184 Columns: 4
## -- Column specification -----
## Delimiter: "\t"
## chr (3): X1, X2, X4
## dbl (1): X3
##
## i Use 'spec()' to retrieve the full column specification for this data.
## i Specify the column types or set 'show_col_types = FALSE' to quiet this message.
## Rows: 10720 Columns: 3
## -- Column specification -----
## Delimiter: ","
## chr (1): variant
## dbl (2): score, pos
##
## i Use 'spec()' to retrieve the full column specification for this data.
## i Specify the column types or set 'show_col_types = FALSE' to quiet this message.
## Rows: 10184 Columns: 15
## -- Column specification -----
## Delimiter: ","
## chr (1): mutant
## dbl (14): column_coverage, popEVE, pop-adjusted_EVE, pop-adjusted_ESM1v, pop...
##
## i Use 'spec()' to retrieve the full column specification for this data.
## i Specify the column types or set 'show_col_types = FALSE' to quiet this message.
## Rows: 10184 Columns: 15
## -- Column specification -----
## Delimiter: ","
## chr (1): mutant
## dbl (14): column_coverage, popEVE, pop-adjusted_EVE, pop-adjusted_ESM1v, pop...
##
## i Use 'spec()' to retrieve the full column specification for this data.
## i Specify the column types or set 'show_col_types = FALSE' to quiet this message.
## Rows: 536 Columns: 27
## -- Column specification -----
## Delimiter: ","

```

```

## chr (15): WT_AA, domains_Pfam, KD_lobe, secondary_structure_uniprot, seconda...
## dbl (1): position
## lgl (11): block1, block2, block3, block4, block5, R-spine, C-spine, Communit...
##
## i Use 'spec()' to retrieve the full column specification for this data.
## i Specify the column types or set 'show_col_types = FALSE' to quiet this message.
## Rows: 4898 Columns: 11
## -- Column specification -----
## Delimiter: ","
## chr (2): id, wt_aa
## dbl (9): FL_kinase_fitness_scaled, FL_kinase_sigma_scaled, FL_abundance_fitn...
##
## i Use 'spec()' to retrieve the full column specification for this data.
## i Specify the column types or set 'show_col_types = FALSE' to quiet this message.
## Running preprocessing script: 04-munge_psd95.R
##
## Sourcing R script: 04-munge_psd95.R
##
## Rows: 3154 Columns: 41
## -- Column specification -----
## Delimiter: ","
## chr (14): id_eve, id_old, trait_name, library, assay, pdz_name, alignment_po...
## dbl (26): X, V1, pos_am, ddg, std_ddg, ci95_kcal.mol, pdz, structural_alignm...
## lgl (1): binding_interface_5A
##
## i Use 'spec()' to retrieve the full column specification for this data.
## i Specify the column types or set 'show_col_types = FALSE' to quiet this message.
## Running preprocessing script: 05-munge-grb2.R
##
## Sourcing R script: 05-munge-grb2.R
##
## Rows: 1056 Columns: 43
## -- Column specification -----
## Delimiter: ","
## chr (15): id, old_id, id_ref, SS, Pos_class, protein, WT_AA, Mut, wt_aa.x, m...
## dbl (23): Pos_real, Pos_ref, Pos, mut_order, f_dg_pred, f_ddg_pred, f_ddg_pr...
## lgl (5): f_ddg_pred_conf, b_ddg_pred_conf, allosteric, orthosteric, alloste...
##
## i Use 'spec()' to retrieve the full column specification for this data.
## i Specify the column types or set 'show_col_types = FALSE' to quiet this message.
## Rows: 1689 Columns: 27
## -- Column specification -----
## Delimiter: ","
## chr (12): id, protein, pca_type, aa_seq, old_id, wt_aa.x, mt_aa, wt_aa.y, at...
## dbl (14): Pos_real, Nham_aa, fitness, sigma, growthrate, growthrate_sigma, c...
## lgl (1): WT
##
## i Use 'spec()' to retrieve the full column specification for this data.
## i Specify the column types or set 'show_col_types = FALSE' to quiet this message.

```

```

gck_abundance <- read.csv("/Users/xl7/Documents/0.Projects/01.protein-seq-evo-v1/data/vampseq/vampseq_d
gck_activity <- read.csv("/Users/xl7/Documents/0.Projects/01.protein-seq-evo-v1/data/vampseq/vampseq_dd
gck_esm <- read.csv("/Users/xl7/Documents/0.Projects/01.protein-seq-evo-v1/data/vampseq/vampseq_esm1v/P
nrow(gck_abundance) #8396

```

```
## [1] 8396
```

```
nrow(gck_activity) #8570
```

```
## [1] 8570
```

```
nrow(gck_esm) #8835
```

```
## [1] 8835
```

```
gck_df <- merge(gck_abundance, gck_esm, by.x = "mutant", by.y = "variant")
gck_df <- gck_df %>% dplyr::select (mutant, DMS_score, DMS_score_bin, ESM.1v) %>%
  dplyr::rename(DMS_score_abundance = DMS_score,
               DMS_score_bin_abundance = DMS_score_bin)
gck_df <- merge(gck_df, gck_activity, by = "mutant")
gck_df <- gck_df %>% dplyr::rename(DMS_score_activity = DMS_score,
               DMS_score_bin_activity = DMS_score_bin) %>%
  dplyr::select (mutant, DMS_score_abundance, DMS_score_bin_abundance, ESM.1v,
               DMS_score_activity, DMS_score_bin_activity)
```

```
gck_df <- gck_df %>%
  mutate(mutation_position = as.numeric(str_extract(mutant, "(?<=\\D)(\\d+)(?=\\D)"))))
gck_clinvar <- read.csv("/Users/xl7/Documents/0.Projects/01.protein-seq-evo-v1/data/vampseq/vampseq_clinvar.csv")
nrow(gck_clinvar) #8835
```

```
## [1] 8835
```

```
gck_df <- merge(gck_df, gck_clinvar, by.x="mutant", by.y="variant")
```

```
gck_clinvar_web <- read.delim("/Users/xl7/Documents/0.Projects/01.protein-seq-evo-v1/data/vampseq/vampseq_clinvar_web.csv")
nrow(gck_clinvar_web) #319
```

```
## [1] 319
```

```
table(gck_clinvar_web$Variant.type)
```

```
##
## single nucleotide variant
##                               319
```

```
# single nucleotide variant
#                               319
```

```
# Map from 3-letter to 1-letter amino acid codes
aa_map <- c(
  Ala="A", Arg="R", Asn="N", Asp="D", Cys="C",
  Gln="Q", Glu="E", Gly="G", His="H", Ile="I",
  Leu="L", Lys="K", Met="M", Phe="F", Pro="P",
  Ser="S", Thr="T", Trp="W", Tyr="Y", Val="V",
```



```

Ter="*"
)

# Extract long-form protein change (e.g., Ala456Val)
gck_clinvar_web$canonical_long <- sub(".*\\(p\\.[A-Za-z]+\\d+[A-Za-z]+\\).*", "\\1", gck_clinvar_web$canonical_long)

# Convert long form to short form using aa_map
gck_clinvar_web$canonical_short <- sapply(gck_clinvar_web$canonical_long, function(change) {
  if (grepl("^[A-Za-z]{3}\\d+[A-Za-z]{3}$", change)) {
    parts <- regmatches(change, regexec("^[A-Za-z]{3}\\d+[A-Za-z]{3}$", change))[[1]]
    from <- aa_map[[parts[2]]]
    to <- aa_map[[parts[4]]]
    pos <- parts[3]
    if (!is.null(from) && !is.null(to)) {
      return(paste0(from, pos, to))
    }
  }
  return(NA)
})

gck_clinvar_web <- gck_clinvar_web %>% dplyr::select( canonical_short, Condition.s., Germline.classification)
nrow(gck_clinvar_web) #319

```

```
## [1] 319
```

```

# Classify based on known pathogenic GCK disease mechanisms
classify_gck_conditions <- function(cond_str) {
  cond_lower <- tolower(cond_str)

  # Individual flags
  is_mody <- grepl("maturity[- ]onset diabetes.*young", cond_lower)
  is_pndm <- grepl("neonatal diabetes", cond_lower)
  is_hh <- grepl("hyperinsulinism", cond_lower)
  is_mono <- grepl("monogenic diabetes", cond_lower)
  is_np <- grepl("not provided", cond_lower)

  # Label assignment based on specific rules
  labels <- c()
  if (is_mody) labels <- c(labels, "MODY")
  if (is_pndm) labels <- c(labels, "PNDM")
  if (is_hh) labels <- c(labels, "HH")
  if (is_mono) labels <- c(labels, "Monogenic diabetes")
  if (is_np && length(labels) == 0) labels <- c("Not provided") # only assign if nothing else detected

  if (length(labels) == 0) {
    return("Other")
  } else if (length(labels) == 1) {
    return(labels)
  } else {
    return("Mixed")
  }
}

```

```
# Apply the classification
gck_clinvar_web$clean_condition <- sapply(gck_clinvar_web$Condition.s., classify_gck_conditions)

# View cleaned summary
#table(gck_clinvar_web$clean_condition)
#HH          Mixed          MODY Monogenic diabetes          Not provided          Other
#3              14              69              189              41              3

gck_clinvar_web <- gck_clinvar_web %>%
  mutate(canonical_short = if_else(
    is.na(canonical_short),
    Protein.change,
    canonical_short
  ))

nrow(gck_clinvar_web) #319 3+14+69+189 = 275
```

```
## [1] 319
```

```
length(unique(gck_clinvar_web$canonical_short)) #313
```

```
## [1] 313
```

```
# Find duplicated canonical_short values
dup_idx <- duplicated(gck_clinvar_web$canonical_short) | duplicated(gck_clinvar_web$canonical_short, fromLast = TRUE)

# Extract rows with duplicated canonical_short values
gck_clinvar_dups <- gck_clinvar_web[dup_idx, ]

gck_clinvar_web <- gck_clinvar_web %>% distinct(canonical_short, .keep_all = TRUE)
nrow(gck_clinvar_web) #313
```

```
## [1] 313
```

```
gck_df_merged <- merge(gck_df, gck_clinvar_web, by.x="mutant", by.y="canonical_short", all.x = TRUE)
nrow(gck_df_merged) #8255
```

```
## [1] 8255
```

```
range(gck_df_merged$DMS_score_abundance) #-0.9834964 1.6096087
```

```
## [1] -0.9834964 1.6096087
```

```
range(gck_df_merged$DMS_score_activity) #-1.085214 6.670528
```

```
## [1] -1.085214 6.670528
```

```
gck_gnomad <- read.csv("/Users/xl7/Documents/0.Projects/01.protein-seq-evo-v1/data/vampseq/vampseq_gnomad.csv")
gck_gnomad <- gck_gnomad %>% filter(VEP.Annotation == "missense_variant")
summary(gck_gnomad$Allele.Frequency)
```

```
##      Min.   1st Qu.   Median     Mean   3rd Qu.     Max.
## 6.195e-07 6.197e-07 6.230e-07 1.099e-05 1.859e-06 2.580e-03
```

```
nrow(gck_gnomad) #528
```

```
## [1] 528
```

```
#      Min.   1st Qu.   Median     Mean   3rd Qu.     Max.
# 6.195e-07 6.197e-07 6.230e-07 1.076e-05 1.859e-06 2.580e-03
```

```
gck_gnomad <- gck_gnomad %>% dplyr::select(HGVS.Consequence, ClinVar.Germline.Classification,
                                           rsIDs, ClinVar.Variation.ID)
nrow(gck_gnomad) #528
```

```
## [1] 528
```

```
# Function to convert e.g. "p.Glu2Gln" → "E2Q"
convert_to_short <- function(consequence) {
  consequence <- gsub("^p\\.\\.", "", consequence) # Remove 'p.'
  matches <- regmatches(consequence, regexec("([A-Za-z]{3})([0-9]+)([A-Za-z]{3})", consequence))[[1]]
  if (length(matches) == 4) {
    from <- aa_map[[matches[2]]]
    pos <- matches[3]
    to <- aa_map[[matches[4]]]
    return(paste0(from, pos, to))
  } else {
    return(NA)
  }
}
```

```
# Apply to the column
gck_gnomad$ID <- sapply(gck_gnomad$HGVS.Consequence, convert_to_short)
nrow(gck_gnomad) #528
```

```
## [1] 528
```

```
length(unique(gck_gnomad$ID)) #519
```

```
## [1] 519
```

```
gck_gnomad <- gck_gnomad %>% distinct(ID, .keep_all = TRUE)
nrow(gck_gnomad) #519
```

```
## [1] 519
```

```
nrow(gck_df_merged) #8255
```

```
## [1] 8255
```

```
gck_df <- merge(gck_df_merged, gck_gnomad, by.x="mutant", by.y = "ID", all.x = TRUE)
nrow(gck_df) #8255
```

```
## [1] 8255
```

```
length(unique(gck_df$mutant)) #8255
```

```
## [1] 8255
```

```
#https://cspec.genome.network/cspec/ui/svi/doc/GN086
active_positions <- c(151:179, # disordered loop
                     151-153, 168-169, 204-206, 225-231, 254-258, 287, 290, # glucose-binding
                     78:85, 151, 169, 205, 225:229, 295:296, 331:333, 336, 410:416 # ATP-binding
)

fil_gck_df <- gck_df %>%
  filter(!mutation_position %in% active_positions)

nrow(fil_gck_df) #7224
```

```
## [1] 7224
```

```
# Fit a loess model using the filtered data
loess_fit <- loess(DMS_score_activity ~ DMS_score_abundance, data = fil_gck_df, span = 0.7, family = "s")

# Predict fitted values for ALL data points using the loess model trained on fil_gck_df
gck_df$fitted <- predict(loess_fit, newdata = gck_df)

# Calculate residuals for ALL points
gck_df$residuals <- gck_df$DMS_score_activity - gck_df$fitted
range(gck_df$residuals) #-1.891487 6.102024
```

```
## [1] -1.891487 6.102024
```

```
# Generate LOESS fit line from fil_gck_df
loess_fit <- loess(DMS_score_activity ~ DMS_score_abundance, data = fil_gck_df, span = 0.7, family = "s")

fit_line_df <- data.frame(
  DMS_score_abundance = seq(-0.6,
                           max(fil_gck_df$DMS_score_abundance, na.rm = TRUE),
                           length.out = 200)
)

fit_line_df$DMS_score_activity <- predict(loess_fit, newdata = fit_line_df)

#length(unique(gck_df$mutant)) #8255

range(gck_df$residuals) #-1.891487 6.102024
```

```
## [1] -1.891487  6.102024
```

```
range(gck_df$DMS_score_abundance) #-0.9834964  1.6096087
```

```
## [1] -0.9834964  1.6096087
```

```
range(gck_df$DMS_score_activity) #-1.085214  6.670528
```

```
## [1] -1.085214  6.670528
```

```
median(gck_df$DMS_score_activity) #0.56
```

```
## [1] 0.5603297
```

```
gck_df <- gck_df %>%  
  mutate(mutation_position = as.numeric(str_extract(mutant, "(?<=\\D)(\\d+)(?=\\D)")))  
nrow(gck_df)
```

```
## [1] 8255
```

```
median_residuals <- gck_df %>%  
  dplyr::group_by(mutation_position) %>%  
  summarise(median_residuals = median(residuals, na.rm = TRUE))  
min(median_residuals$median_residuals) #-1.136173
```

```
## [1] -1.136173
```

```
max(median_residuals$median_residuals) #2.551111
```

```
## [1] 2.551111
```

```
pdb <- read.pdb("/Users/xl7/Documents/0.Projects/01.protein-seq-evo-v1/data/residual_pdb/GCK/1v4s.pdb")  
data <- median_residuals  
head(data)
```

```
## # A tibble: 6 x 2  
##   mutation_position median_residuals  
##           <dbl>           <dbl>  
## 1             2             0.135  
## 2             3             0.336  
## 3             4             0.369  
## 4             5             0.0300  
## 5             6            -0.0184  
## 6             7             0.245
```

```

# Create a new B-factor vector initialized with the current B-factors from the PDB
new_b_factors <- pdb$atom$b

# Loop through each position in the correlation data and update the B-factors
for (i in 1:nrow(data)) {
  position <- data$mutation_position[i]
  correlation_value <- data$median_residuals[i]

  # Find indices in the PDB that match the current position
  indices <- which(pdb$atom$resno == position)

  # Print the indices and current B-factors before updating
  #cat("Updating residue number:", position, "\n")
  #cat("Indices in PDB:", indices, "\n")
  #cat("Current B-factors:", new_b_factors[indices], "\n")

  # Update B-factors for all atoms in the current residue
  new_b_factors[indices] <- correlation_value

  # Print the new B-factors after updating
  #cat("Updated B-factors:", new_b_factors[indices], "\n")
  #cat("\n") # Add an extra line for readability
}

# Replace non-matching B-factors with outlier value so we can filter it out in ChimeraX
non_matching_indices <- setdiff(seq_along(new_b_factors), which(pdb$atom$resno %in% data$mutation_position))
new_b_factors[non_matching_indices] <- 999

# Assign the new B-factors back to the pdb structure
# Write the modified PDB structure to a new file
pdb$atom$b <- new_b_factors
write.pdb(pdb, file = "/Users/xl7/Documents/0.Projects/01.protein-seq-evo-v1/data/residual_pdb/GCK/1v4s.pdb")

# Plot
nrow(gck_df)

```

```
## [1] 8255
```

```

p1 <- ggplot(gck_df, aes(x = DMS_score_abundance, y = DMS_score_activity, color = residuals)) +
  geom_point(size = 2, alpha = 0.35) +
  geom_vline(xintercept = 0.58, linetype = "dashed", linewidth = 0.5, color = "grey") +
  geom_hline(yintercept = 0.66, linetype = "dashed", linewidth = 0.5, color = "grey") +
  geom_line(data = fit_line_df, aes(x = DMS_score_abundance, y = DMS_score_activity),
            inherit.aes = FALSE, color = "black", linewidth = 1) +
  geom_text_repel(data = subset(gck_df, mutant %in% c("Y214E")),
                  aes(label = mutant),
                  size = 4, color = "gold2",
                  max.overlaps = Inf, box.padding = 0.4, point.padding = 0.3
  ) +
  geom_text_repel(data = subset(gck_df, mutant %in% c("T206M", "V452L")),
                  aes(label = mutant),
                  size = 4, color = "black",
                  max.overlaps = Inf, box.padding = 0.4, point.padding = 0.3
  ) +

```

```

geom_point(data = subset(gck_df, mutant %in% c("T206M", "V452L")),
  aes(x = DMS_score_abundance, y = DMS_score_activity),
  shape = 17, color = "black", size = 3) + # Triangle shape
scale_color_viridis(option = "C", direction = 1, limits = c(-6.2, 6.2)) +
labs(
  title = "All 8255 Variants",
  x = "Measured abundance",
  y = "Measured activity",
  color = "LOESS residuals"
) +
scale_y_continuous(breaks = seq(-1, 7, by = 2)) + xlim(-1, 1.7) +
theme_classic() + theme(legend.position = "none") + theme(
  panel.background = element_rect(fill = "white", color = NA),
  plot.background = element_rect(fill = "white", color = NA),
  legend.background = element_rect(fill = "white", color = NA)
)

p1 <- ggMarginal(
  p1,
  type = "density",
  margins = "both",
  groupColour = FALSE,
  groupFill = FALSE,
  size = 10,
  colour = "grey",
  fill = "lightgrey"
)

patho_df <- gck_df %>% filter(!is.na(Germline.classification))
#nrow(patho_df) #277

p2 <- ggplot(patho_df, aes(x = DMS_score_abundance, y = DMS_score_activity, color = residuals)) +
  geom_point(size = 2, shape = 17) +
  geom_text_repel(data = subset(gck_df, mutant %in% c("T206M", "V452L")),
    aes(label = mutant),
    size = 4, color = "black",
    max.overlaps = Inf, box.padding = 0.4, point.padding = 0.3
  ) +
  geom_point(data = subset(gck_df, mutant %in% c("T206M", "V452L")),
    aes(x = DMS_score_abundance, y = DMS_score_activity),
    shape = 17, color = "black", size = 3) + # Triangle shape
  geom_vline(xintercept = 0.58, linetype = "dashed", linewidth = 0.5, color = "grey") +
  geom_hline(yintercept = 0.66, linetype = "dashed", linewidth = 0.5, color = "grey") +
  geom_line(data = fit_line_df, aes(x = DMS_score_abundance, y = DMS_score_activity),
    inherit.aes = FALSE, color = "black", linewidth = 1) +
  scale_color_viridis(option = "C", direction = 1, limits = c(-6.2, 6.2)) +
  labs(
    title = "ClinVar Pathogenic Variants",
    x = "Measured abundance",
    y = "Measured activity",
    color = "Loess residuals"
  ) + scale_y_continuous(
    breaks = seq(-1, 7, by = 2),

```

```

    limits = c(-1.1, 7)
  ) +
  theme_classic() + xlim(-1,1.7) +
  theme(legend.position = "none")

p2 <- ggMarginal(
  p2,
  type = "density",
  margins = "both",
  groupColour = FALSE,
  groupFill = FALSE,
  size = 10,
  colour = "grey",
  fill = "lightgrey"
)

gnomad_df <- gck_df %>% filter(!is.na(HGVS.Consequence)) %>%
  filter(!clinvar_clinical_significance %in% c("likely_pathogenic", "pathogenic", "conflict", "likely_r
  filter(!ClinVar.Germline.Classification %in% c("Pathogenic", "Pathogenic/Likely pathogenic", "Likely p
    "Conflicting classifications of pathogenicity", "Likely
    "Likely risk allele", "Pathogenic/Likely pathogenic/Lil
    "Uncertain significance", "Uncertain significance/Uncer

  filter(is.na(Germline.classification))
  #filter(is.na(Phenotype_Class))
  #filter(is.na(somatic))

#nrow(gnomad_df) #268

p3 <- ggplot(gnomad_df, aes(x = DMS_score_abundance, y = DMS_score_activity, color = residuals)) +
  geom_point(size = 2) +
  geom_vline(xintercept = 0.58, linetype = "dashed", linewidth = 0.5, color = "grey") +
  geom_hline(yintercept = 0.66, linetype = "dashed", linewidth = 0.5, color = "grey") +
  geom_line(data = fit_line_df, aes(x = DMS_score_abundance, y = DMS_score_activity),
    inherit.aes = FALSE, color = "black", linewidth = 1) +
  geom_text_repel(data = subset(gck_df, mutant %in% c("A11T", "E279Q", "R46K")),
    aes(label = mutant),
    size = 4, color = "black",
    max.overlaps = Inf, box.padding = 0.4, point.padding = 0.3
  ) +
  geom_point(data = subset(gck_df, mutant %in% c("A11T", "E279Q", "R46K")),
    aes(x = DMS_score_abundance, y = DMS_score_activity),
    color = "black", size = 2) + # Triangle shape
  scale_color_viridis(option = "C", direction = 1, limits = c(-6.2, 6.2)) +
  labs(
    title = "gnomAD Variants",
    x = "Measured abundance",
    y = "Measured activity",
    color = "Loess residuals"
  ) + theme_classic() + scale_y_continuous(breaks = seq(-1, 7, by = 2),
    limits = c(-1, 7)) + xlim(-1,1.7) + theme(legend.position = "none")

```



```

p3 <- ggMarginal(
  p3,
  type = "density",
  margins = "both",
  groupColour = FALSE,
  groupFill = FALSE,
  size = 10,
  colour = "grey",
  fill = "lightgrey"
)

benign_df <- gck_df %>%
  filter(clinvar_clinical_significance %in% c("likely_benign", "benign")) %>%
  filter(!ClinVar.Germline.Classification %in% c("Pathogenic", "Pathogenic/Likely pathogenic", "Likely pathogenic", "Likely pathogenic of pathogenicity", "Conflicting classifications of pathogenicity")) %>%
  filter(is.na(Germline.classification))

#nrow(benign_df) #3

p4 <- ggplot(benign_df, aes(x = DMS_score_abundance, y = DMS_score_activity, color = residuals)) +
  geom_point(size = 2) +
  geom_vline(xintercept = 0.58, linetype = "dashed", linewidth = 0.5, color = "grey") +
  geom_hline(yintercept = 0.66, linetype = "dashed", linewidth = 0.5, color = "grey") +
  geom_line(data = fit_line_df, aes(x = DMS_score_abundance, y = DMS_score_activity),
    inherit.aes = FALSE, color = "black", linewidth = 1) +
  scale_color_viridis(option = "C", direction = 1, limits = c(-6.2, 6.2)) +
  labs(
    title = "ClinVar Benign Variants",
    x = "Measured abundance",
    y = "Measured activity",
    color = "Loess residuals"
  ) + theme_classic() + scale_y_continuous(breaks = seq(-1, 7, by = 2),
    limits = c(-1, 7)) + xlim(-1, 1.7) + theme(legend.position = "bottom")

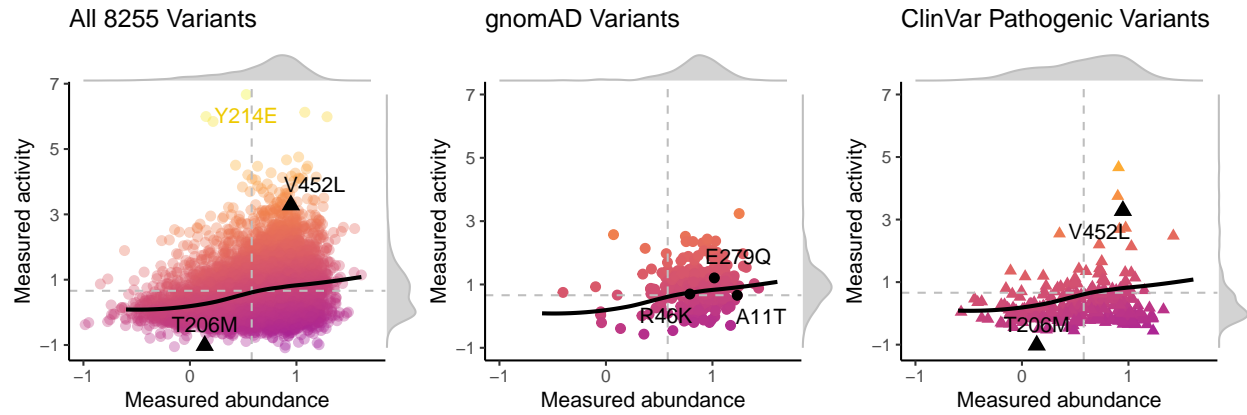
p4 <- ggMarginal(
  p4,
  type = "density",
  margins = "both",
  groupColour = FALSE,
  groupFill = FALSE,
  size = 10,
  colour = "grey",
  fill = "lightgrey"
)

p5 <- plot_grid(p1, p3, p2, nrow=1, ncol=3)

ggsave("/Users/xl7/Documents/0.Projects/01.protein-seq-evo-v1/figs/panels/fig5_scatter.pdf",
  plot = p5, width = 9, height = 3, dpi = 300)

p5

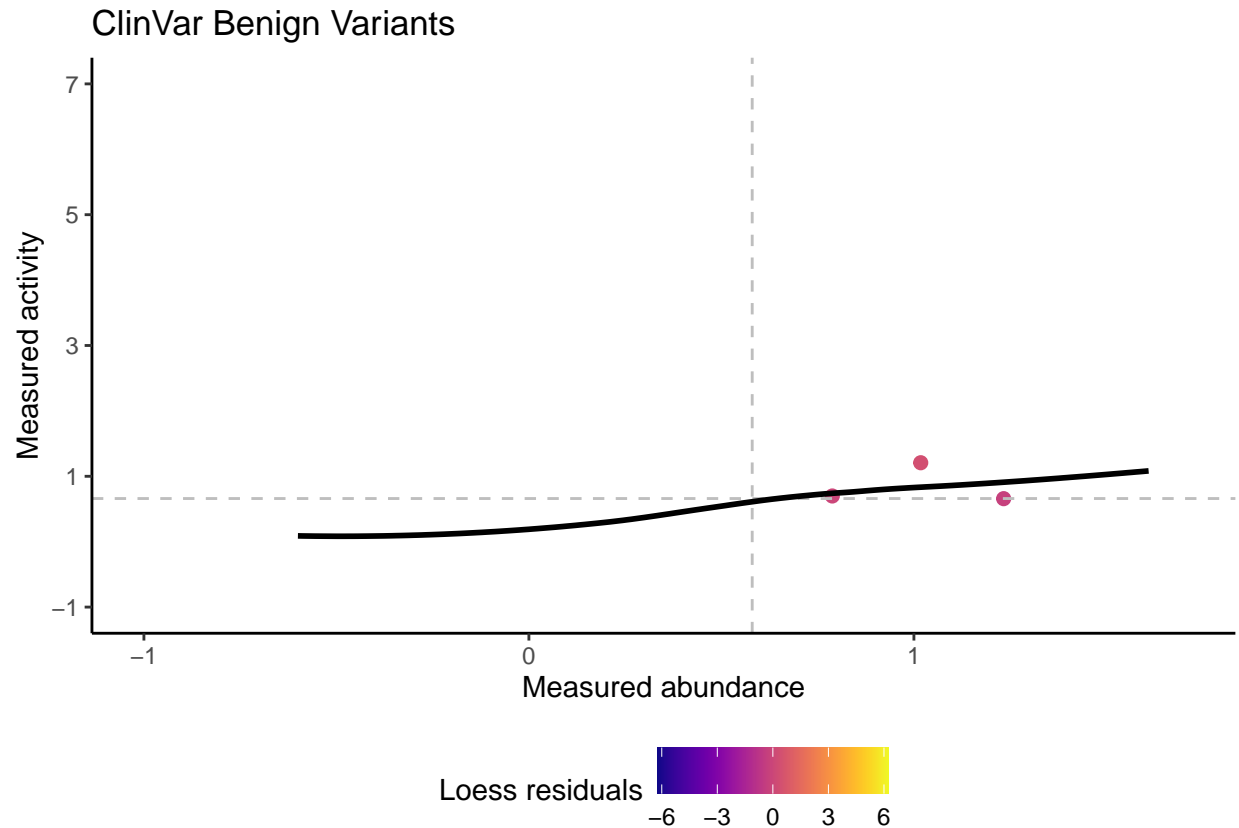
```



```
p1 <- ggplot(benign_df, aes(x = DMS_score_abundance, y = DMS_score_activity, color = residuals)) +
  geom_point(size = 2) +
  geom_vline(xintercept = 0.58, linetype = "dashed", linewidth = 0.5, color = "grey") +
  geom_hline(yintercept = 0.66, linetype = "dashed", linewidth = 0.5, color = "grey") +
  geom_line(data = fit_line_df, aes(x = DMS_score_abundance, y = DMS_score_activity),
    inherit.aes = FALSE, color = "black", linewidth = 1) +
  scale_color_viridis(option = "C", direction = 1, limits = c(-6.2, 6.2)) +
  labs(
    title = "ClinVar Benign Variants",
    x = "Measured abundance",
    y = "Measured activity",
    color = "Loess residuals"
  ) + theme_classic() + scale_y_continuous(breaks = seq(-1, 7, by = 2),
    limits = c(-1, 7)) + xlim(-1, 1.7) +
  theme(legend.position = "bottom")

ggsave("/Users/xl7/Documents/0.Projects/01.protein-seq-evo-v1/figs/panels/fig5_scatter_legend.pdf",
  plot = p1, width = 3, height = 3, dpi = 300)

p1
```



```
# 1. Set up
set.seed(123)
n_boot <- 1000
match_window <- 0.05
n_patho <- nrow(patho_df)

# 2. Get abundance/residuals from gck_patho
patho_df <- patho_df %>% dplyr::select(DMS_score_abundance, residuals)
patho_df$group <- "Pathogenic"

# 3. Bootstrap sampling from non-patho pool with abundance matching
non_patho_pool <- gck_df %>%
  filter(!(mutant %in% patho_df$mutant))

bootstrap_medians <- vector("numeric", length = n_boot)

# Pre-group non-patho pool into bins
non_patho_pool <- non_patho_pool %>%
  mutate(bin = cut(DMS_score_abundance, breaks = seq(-0.5, 2, by = match_window)))

# Bin pathogenic variants accordingly
patho_df <- patho_df %>%
  mutate(bin = cut(DMS_score_abundance, breaks = seq(-0.5, 2, by = match_window)))

# Create lookup table for fast sampling
bin_lookup <- split(non_patho_pool$residuals, non_patho_pool$bin)
```

```

# Bootstrap matrix
bootstrap_matrix <- matrix(NA, nrow = n_boot, ncol = n_patho)

for (i in 1:n_boot) {
  for (j in 1:n_patho) {
    bin_j <- patho_df$bin[j]
    candidates <- bin_lookup[[as.character(bin_j)]]
    if (!is.null(candidates) && length(candidates) > 0) {
      bootstrap_matrix[i, j] <- sample(candidates, 1)
    }
  }
}

# Summarize into a dataframe
boot_df <- data.frame(
  group = "Random abundance-matched",
  residuals = apply(bootstrap_matrix, 1, median, na.rm = TRUE)
)

# Combine with patho residuals
plot_df <- bind_rows(
  patho_df %>% dplyr::select(group, residuals),
  boot_df
)

label_df <- plot_df %>%
  group_by(group) %>%
  summarise(
    n = n(),
    median_val = median(residuals),
    y_max = max(residuals),
    .groups = "drop"
  )

label_df <- label_df %>%
  mutate(n_label = case_when(
    group == "Random abundance-matched" ~ "bootstrapped 1000 times",
    TRUE ~ paste0("n = ", n)
  ))

# Plot
p_fast <- ggplot(plot_df, aes(x = group, y = residuals, fill = group)) +
  geom_violin(trim = FALSE, scale = "width", alpha = 0.8, color = NA) +
  geom_jitter(width = 0.15, size = 2, alpha = 0.7, color = "lightgrey") +
  stat_summary(fun = median, geom = "crossbar", width = 0.4, color = "black", fatten = 1) +
  stat_summary(fun = median, geom = "point", shape = 23, size = 2.5,
    fill = "black", color = "black", stroke = 0.7) +

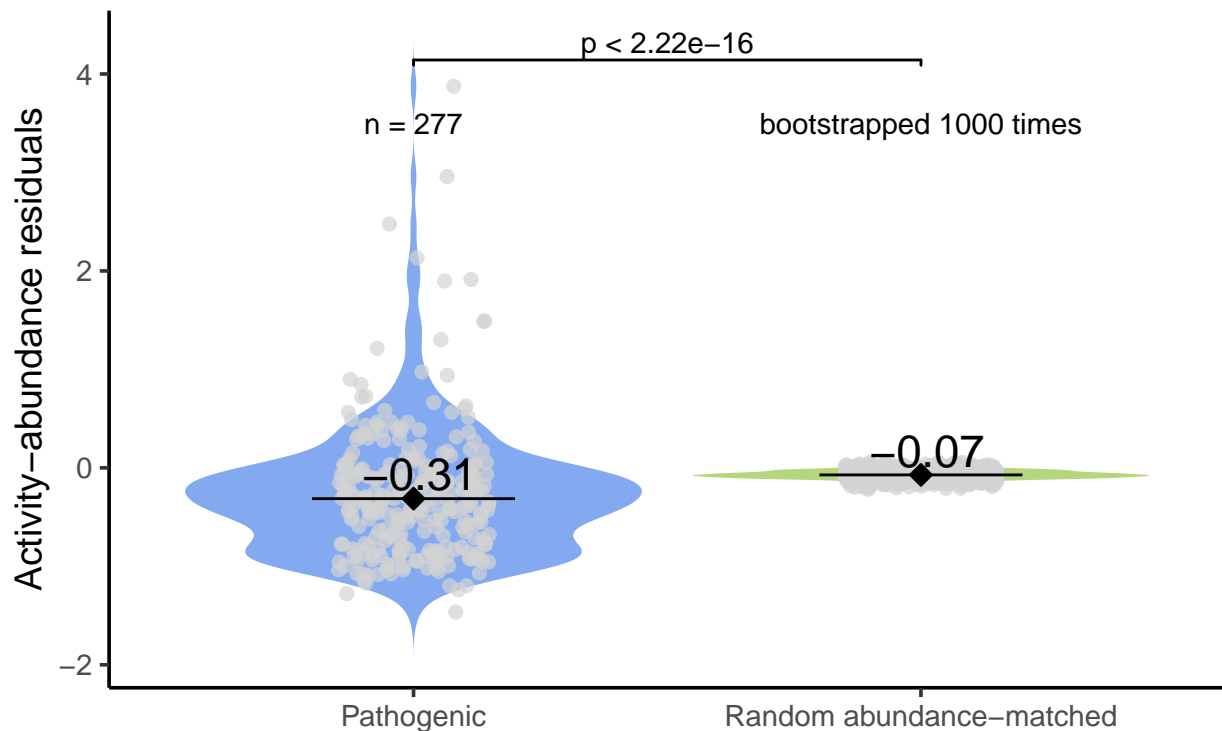
  geom_text(
    data = label_df,
    aes(x = group, y = 3.5, label = n_label),
    inherit.aes = FALSE,
    size = 4) +

```

```

geom_text(
  data = label_df,
  aes(x = group, y = median_val + 0.25, label = sprintf(" %.2f", median_val)),
  inherit.aes = FALSE,
  size = 6
) +
labs(
  x = "",
  y = "Activity-abundance residuals",
  title = ""
) +
theme_classic(base_size = 14) +
scale_fill_manual(values = c("Pathogenic" = "cornflowerblue", "Random abundance-matched" = "darkolivegreen3"),
  theme(legend.position = "none") +
geom_signif(comparisons = list(c("Pathogenic", "Random abundance-matched")),
  map_signif_level = FALSE,
  test = "wilcox.test",
  tip_length = 0.01)
p_fast

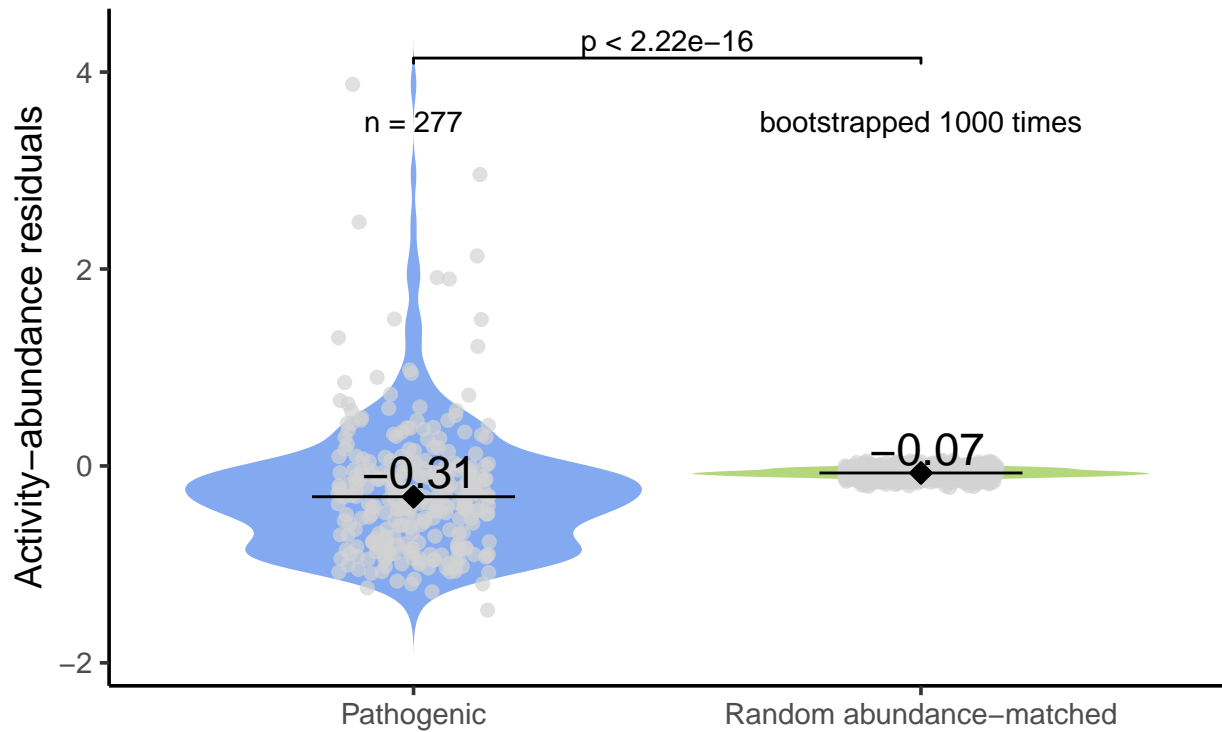
```



```

ggsave("/Users/xl7/Documents/01.Projects/01.protein-seq-evo-v1/figs/panels/fig5_violin1.pdf",
  plot = p_fast, width = 3, height = 4, dpi = 300)
p_fast

```



```
nrow(gnomad_df) #268
```

```
## [1] 268
```

```
patho_df <- gck_df %>% filter(!is.na(Germline.classification))
#nrow(patho_df) #277
gnomad_df <- gnomad_df %>% dplyr::select(mutant, DMS_score_abundance, DMS_score_activity, residuals)
patho_df1 <- patho_df %>% filter(clean_condition == "HH") %>% dplyr::select(mutant, DMS_score_abundance, DMS_score_activity, residuals)
patho_df2 <- patho_df %>% filter(clean_condition == "MODY") %>% dplyr::select(mutant, DMS_score_abundance, DMS_score_activity, residuals)
patho_df3 <- patho_df %>% filter(clean_condition == "Monogenic diabetes") %>% dplyr::select(mutant, DMS_score_abundance, DMS_score_activity, residuals)
nrow(patho_df1)
```

```
## [1] 3
```

```
nrow(patho_df2)
```

```
## [1] 57
```

```
nrow(patho_df3)
```

```
## [1] 164
```

```

patho_df1$var_class2 <- "HH"
patho_df2$var_class2 <- "MODY"
patho_df3$var_class2 <- "Monogenic diabetes"
gnomad_df$var_class2 <- "gnomAD"

```

```
wilcox.test(patho_df1$residuals, gnomad_df$residuals) #0.004004
```

```

##
## Wilcoxon rank sum test with continuity correction
##
## data: patho_df1$residuals and gnomad_df$residuals
## W = 791, p-value = 0.004004
## alternative hypothesis: true location shift is not equal to 0

```

```
wilcox.test(patho_df2$residuals, gnomad_df$residuals) #3.87e-07
```

```

##
## Wilcoxon rank sum test with continuity correction
##
## data: patho_df2$residuals and gnomad_df$residuals
## W = 4368, p-value = 3.87e-07
## alternative hypothesis: true location shift is not equal to 0

```

```
wilcox.test(patho_df3$residuals, gnomad_df$residuals) #< 2.2e-16
```

```

##
## Wilcoxon rank sum test with continuity correction
##
## data: patho_df3$residuals and gnomad_df$residuals
## W = 10458, p-value < 2.2e-16
## alternative hypothesis: true location shift is not equal to 0

```

```
wilcox.test(patho_df1$residuals, patho_df2$residuals) #0.003939
```

```

##
## Wilcoxon rank sum test with continuity correction
##
## data: patho_df1$residuals and patho_df2$residuals
## W = 171, p-value = 0.003939
## alternative hypothesis: true location shift is not equal to 0

```

```
wilcox.test(patho_df1$residuals, patho_df3$residuals) #0.003479
```

```

##
## Wilcoxon rank sum test with continuity correction
##
## data: patho_df1$residuals and patho_df3$residuals
## W = 489, p-value = 0.003479
## alternative hypothesis: true location shift is not equal to 0

```

```
wilcox.test(patho_df2$residuals, patho_df3$residuals) #0.3465
```

```
##
## Wilcoxon rank sum test with continuity correction
##
## data: patho_df2$residuals and patho_df3$residuals
## W = 5066, p-value = 0.3465
## alternative hypothesis: true location shift is not equal to 0
```

```
combined_df <- rbind(patho_df1,patho_df2,patho_df3,gnomad_df)
median_df <- combined_df %>%
  group_by(var_class2) %>%
  summarise(
    median_residual = median(residuals),
    n = n()
  )
median_df
```

```
## # A tibble: 4 x 3
##   var_class2      median_residual      n
##   <chr>          <dbl> <int>
## 1 HH              1.90      3
## 2 MODY            -0.313     57
## 3 Monogenic diabetes -0.359    164
## 4 gnomAD           0.151    268
```

```
combined_df$var_class2 <- factor(
  combined_df$var_class2,
  levels = c("gnomAD", "HH", "MODY", "Monogenic diabetes")
)
```

```
custom_colors <- c(
  "gnomAD" = "#1b9e77", # Teal green
  "HH" = "#f4a6b3", # Warm orange
  "MODY" = "#e7298a", # Muted purple
  "Monogenic diabetes" = "#7570b3" # Hot pink / magenta
)
```

```
p10 <- ggplot(combined_df, aes(x = var_class2, y = residuals, fill = var_class2)) +
  geom_violin(trim = FALSE, scale = "width", alpha = 0.8, color = NA) +
  geom_jitter(width = 0.15, size = 2, alpha = 0.7, color = "lightgrey") +
  stat_summary(fun = median, geom = "crossbar", width = 0.4, color = "black", fatten = 1) +
  stat_summary(fun = median, geom = "point", shape = 23, size = 2, fill = "black", color = "black", stroke = "black") +
  geom_text(
    data = median_df,
    aes(x = var_class2, y = median_residual + 0.5, label = sprintf("%.2f", median_residual)),
    inherit.aes = FALSE,
    size = 5
  ) +
  scale_fill_manual(values = custom_colors) +
  geom_text(
    data = median_df,
```

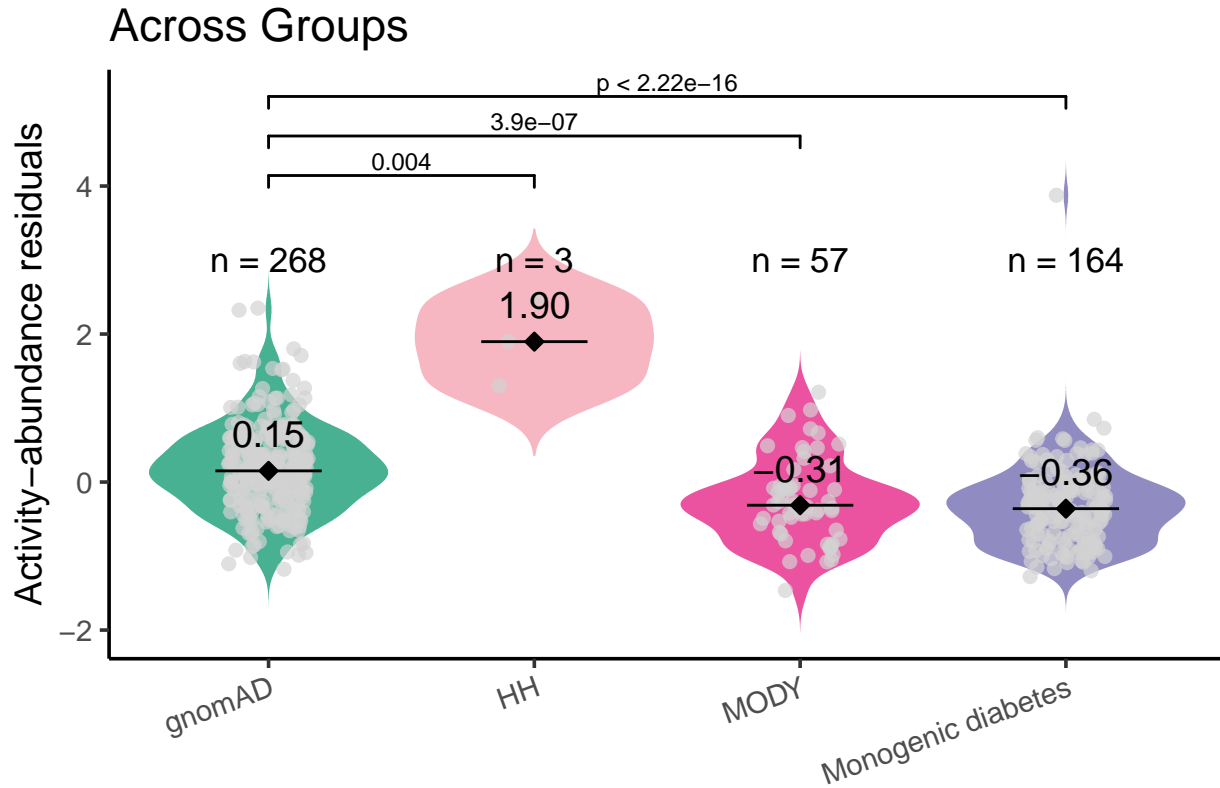


```

aes(x = var_class2, y = 3, label = paste0("n = ", n)),
inherit.aes = FALSE,
size = 4.5
) +
labs(
  title = "Across Groups",
  x = "",
  y = "Activity-abundance residuals",
  fill = ""
) +
theme_classic(base_size = 14) +
theme(
  legend.position = "none",
  axis.text.x = element_text(angle = 20, hjust = 1)
) +
geom_signif(
  comparisons = list(c("gnomAD", "HH"),
                    c("gnomAD", "MODY"),
                    c("gnomAD", "Monogenic diabetes")),
  map_signif_level = FALSE,
  test = "wilcox.test",
  step_increase = 0.1,
  textsize = 3
)

ggsave("/Users/xl7/Documents/0.Projects/01.protein-seq-evo-v1/figs/panels/fig5_violin2.pdf",
        plot = p10, width = 3, height = 4, dpi = 300)
p10

```



```
#nrow(gnomad_df) #268
#nrow(patho_df) #277
#length(unique(patho_df$mutant)) #277
#table(patho_df$clean_condition)
#HH          Mixed          MODY Monogenic diabetes    Not provided    Other
#3           14           57          164           36           3

patho_df <- patho_df %>% filter(clean_condition %in% c("HH", "MODY", "Monogenic diabetes"))
gnomad_df$var_source <- "gnomAD"
patho_df$var_source <- "Pathogenic"

gnomad_df <- gnomad_df %>% dplyr::select(mutant, residuals, var_source, DMS_score_abundance)
patho_df <- patho_df %>% dplyr::select(mutant, residuals, var_source, DMS_score_abundance)

combined_df <- rbind(gnomad_df, patho_df)

combined_df <- combined_df %>%
  mutate(mutation_position = as.numeric(str_extract(mutant, "(?<=\\D)(\\d+)(?=\\D)")))

combined_df_int <- combined_df %>% filter(mutation_position %in% active_positions)
nrow(combined_df_int) #71

## [1] 71
```

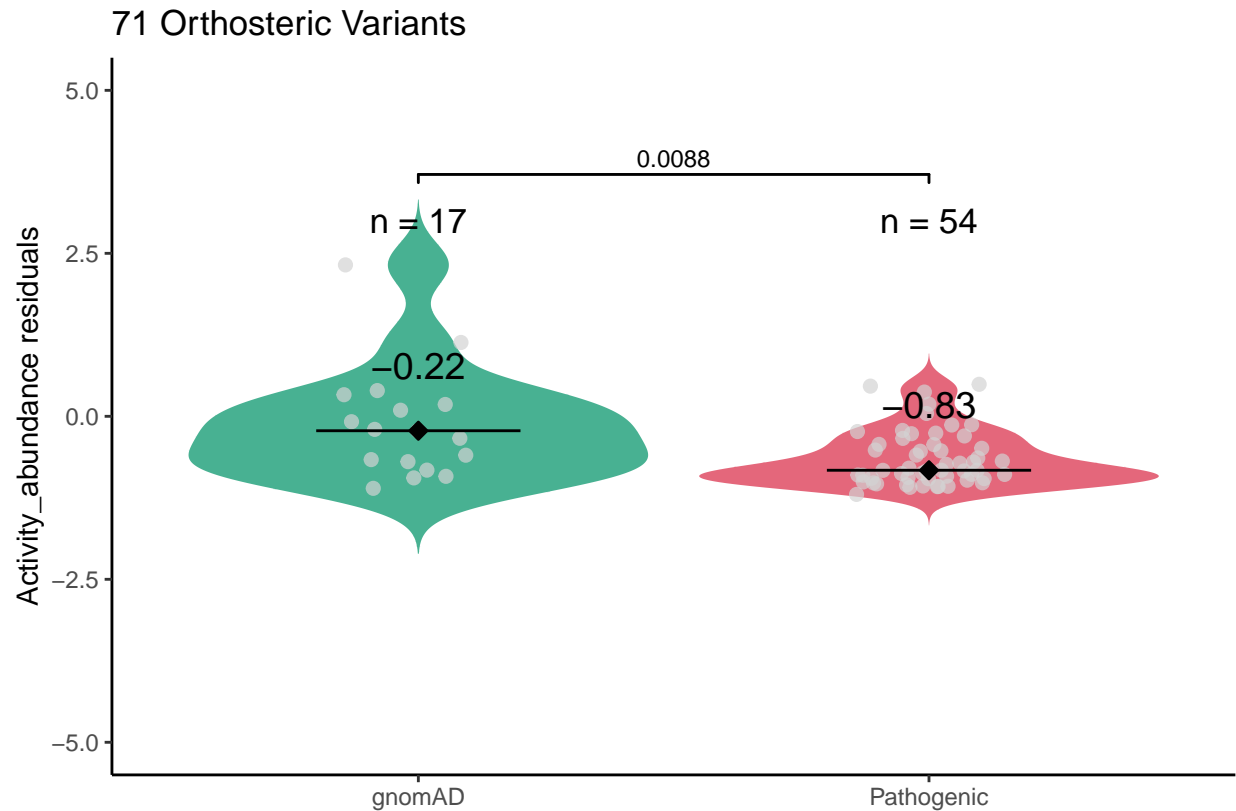
```

#length(unique(combined_df_int$mutant)) #71

median_df <- combined_df_int %>%
  group_by(var_source) %>%
  summarise(
    median_residual = median(residuals, na.rm = TRUE),
    n = n()
  )
#median_df

#table(combined_df_int$var_source)
custom_colors <- c(
  "gnomAD" = "#1b9e77", # Teal green (unchanged)
  "Pathogenic" = "#de425b" # Deep ocean blue
)
p13 <- ggplot(combined_df_int, aes(x = var_source, y = residuals, fill = var_source)) +
  geom_violin(trim = FALSE, scale = "width", alpha = 0.8, color = NA) +
  geom_jitter(width = 0.15, size = 2, alpha = 0.7, color = "lightgrey") +
  stat_summary(fun = median, geom = "crossbar", width = 0.4, color = "black", fatten = 1) +
  stat_summary(fun = median, geom = "point", shape = 23, size = 2, fill = "black", color = "black", stroke = "black") +
  geom_text(
    data = median_df,
    aes(x = var_source, y = median_residual + 1, label = sprintf("%.2f", median_residual)),
    inherit.aes = FALSE,
    size = 5
  ) +
  scale_fill_manual(values = custom_colors) +
  geom_text(
    data = median_df,
    aes(x = var_source, y = 3, label = paste0("n = ", n)),
    inherit.aes = FALSE,
    size = 4.5
  ) +
  labs(
    title = "71 Orthosteric Variants",
    x = "",
    y = "Activity_abundance residuals",
    fill = ""
  ) +
  theme_classic() +
  theme(
    legend.position = "none"
  ) +
  geom_signif(
    comparisons = list(c("gnomAD", "Pathogenic")),
    map_signif_level = FALSE,
    test = "wilcox.test",
    step_increase = 0.1, y_position = 3.5,
    textsize = 3
  ) + ylim(-5, 5)
p13

```



```
combined_df_out <- combined_df %>% filter(!mutation_position %in% active_positions)
nrow(combined_df_out) #421
```

```
## [1] 421
```

```
median_df <- combined_df_out %>%
  group_by(var_source) %>%
  summarise(
    median_residual = median(residuals, na.rm = TRUE),
    n = n()
  )
#median_df

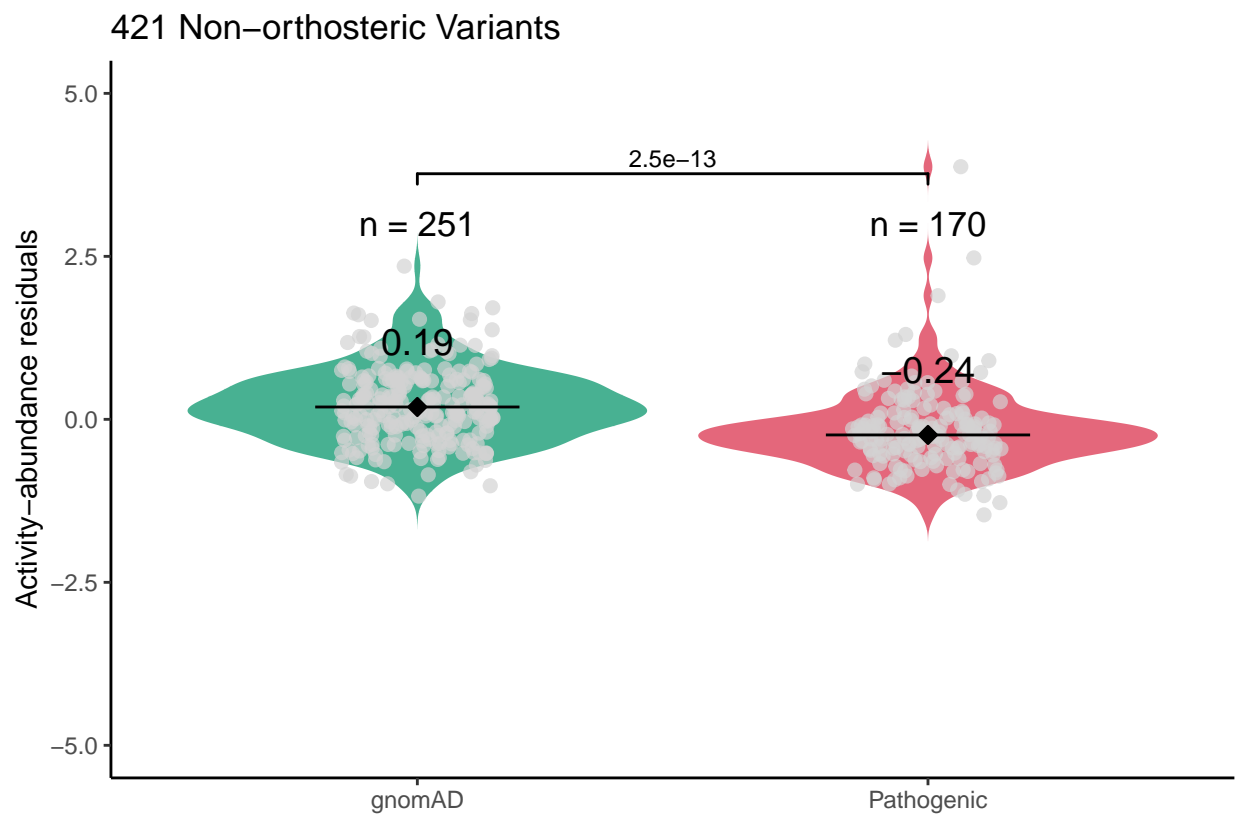
p14 <- ggplot(combined_df_out, aes(x = var_source, y = residuals, fill = var_source)) +
  geom_violin(trim = FALSE, scale = "width", alpha = 0.8, color = NA) +
  geom_jitter(width = 0.15, size = 2, alpha = 0.7, color = "lightgrey") +
  stat_summary(fun = median, geom = "crossbar", width = 0.4, color = "black", fatten = 1) +
  stat_summary(fun = median, geom = "point", shape = 23, size = 2, fill = "black", color = "black", stroke = "black") +
  geom_text(
    data = median_df,
    aes(x = var_source, y = median_residual + 1, label = sprintf("%.2f", median_residual)),
    inherit.aes = FALSE,
    size = 5
  ) +
  scale_fill_manual(values = custom_colors) +
```

```

geom_text(
  data = median_df,
  aes(x = var_source, y = 3, label = paste0("n = ", n)),
  inherit.aes = FALSE,
  size = 4.5
) +
labs(
  title = "421 Non-orthosteric Variants",
  x = "",
  y = "Activity-abundance residuals",
  fill = ""
) +
theme_classic() +
theme(
  legend.position = "none"
) +
geom_signif(
  comparisons = list(c("gnomAD", "Pathogenic")),
  map_signif_level = FALSE,
  test = "wilcox.test",
  step_increase = 0.1, y_position = 3.5,
  textsize = 3
) + ylim(-5, 5)

```

p14



```
combined_df_stable <- combined_df %>% filter(DMS_score_abundance > 0.58)
nrow(combined_df_stable) #350
```

```
## [1] 350
```

```
#table(combined_df_stable$var_source)
```

```
combined_df_stable_int <- combined_df_stable %>% filter(mutation_position %in% active_positions)
nrow(combined_df_stable_int) #59
```

```
## [1] 59
```

```
median_df <- combined_df_stable_int %>%
  group_by(var_source) %>%
  summarise(
    median_residual = median(residuals, na.rm = TRUE),
    n = n()
  )
```

```
#median_df
```

```
p15 <- ggplot(combined_df_stable_int, aes(x = var_source, y = residuals, fill = var_source)) +
  geom_violin(trim = FALSE, scale = "width", alpha = 0.8, color = NA) +
  geom_jitter(width = 0.15, size = 2, alpha = 0.7, color = "lightgrey") +
  stat_summary(fun = median, geom = "crossbar", width = 0.4, color = "black", fatten = 1) +
  stat_summary(fun = median, geom = "point", shape = 23, size = 2, fill = "black", color = "black", stroke = "black") +
  geom_text(
    data = median_df,
    aes(x = var_source, y = median_residual + 1, label = sprintf("%.2f", median_residual)),
    inherit.aes = FALSE,
    size = 5
  ) +
  scale_fill_manual(values = custom_colors) +
  geom_text(
    data = median_df,
    aes(x = var_source, y = 3, label = paste0("n = ", n)),
    inherit.aes = FALSE,
    size = 4.5
  ) +
  labs(
    title = "59 WT-abundance Orthosteric Variants",
    x = "",
    y = "Activity-abundance residuals",
    fill = ""
  ) +
  theme_classic() +
  theme(
    legend.position = "none"
  ) +
  geom_signif(
    comparisons = list(c("gnomAD", "Pathogenic")),
    map_signif_level = FALSE,
    test = "wilcox.test",
```

```

    step_increase = 0.1, y_position = 3.5,
    textsize = 3
) + ylim(-5, 5)

combined_df_stable_out <- combined_df_stable %>% filter(!mutation_position %in% active_positions)
nrow(combined_df_stable_out) #291

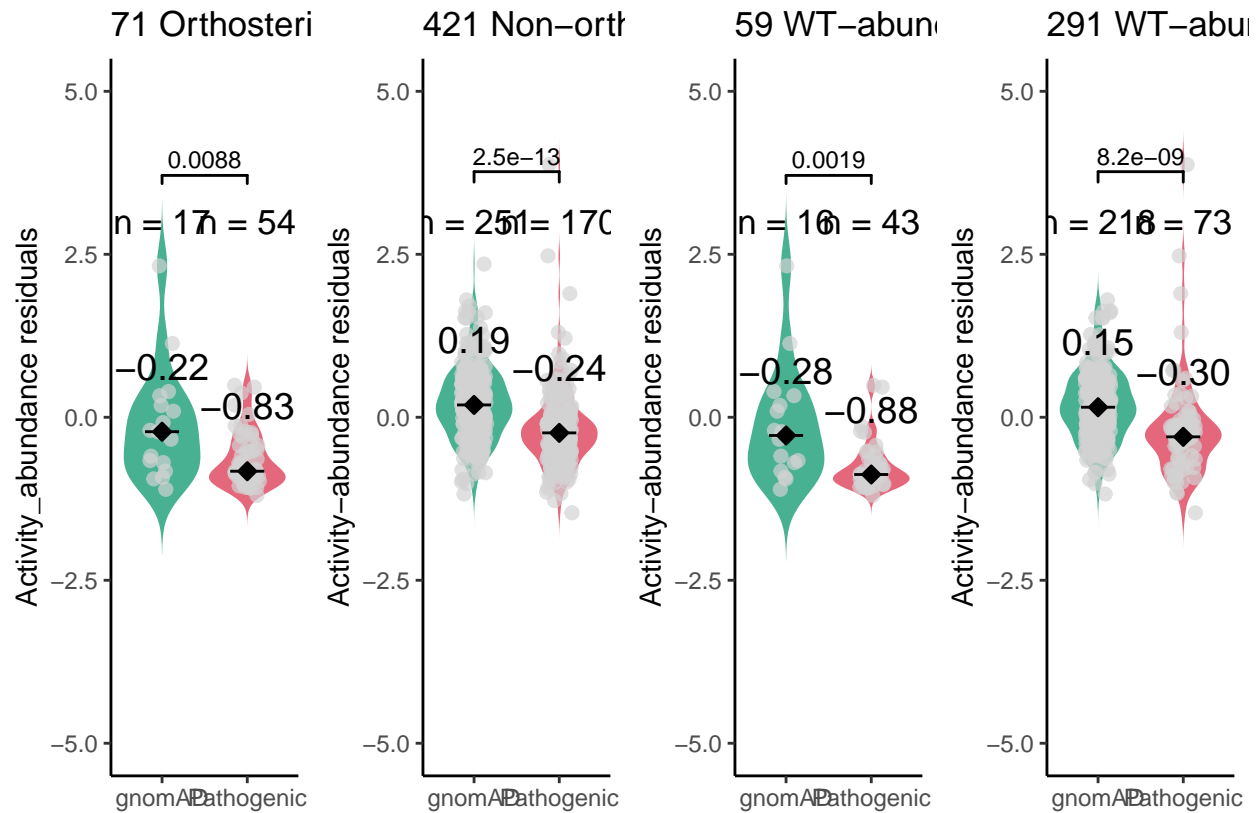
## [1] 291

median_df <- combined_df_stable_out %>%
  group_by(var_source) %>%
  summarise(
    median_residual = median(residuals, na.rm = TRUE),
    n = n()
  )
#median_df

p16 <- ggplot(combined_df_stable_out, aes(x = var_source, y = residuals, fill = var_source)) +
  geom_violin(trim = FALSE, scale = "width", alpha = 0.8, color = NA) +
  geom_jitter(width = 0.15, size = 2, alpha = 0.7, color = "lightgrey") +
  stat_summary(fun = median, geom = "crossbar", width = 0.4, color = "black", fatten = 1) +
  stat_summary(fun = median, geom = "point", shape = 23, size = 2, fill = "black", color = "black", stroke = "black") +
  geom_text(
    data = median_df,
    aes(x = var_source, y = median_residual + 1, label = sprintf("%.2f", median_residual)),
    inherit.aes = FALSE,
    size = 5
  ) +
  scale_fill_manual(values = custom_colors) +
  geom_text(
    data = median_df,
    aes(x = var_source, y = 3, label = paste0("n = ", n)),
    inherit.aes = FALSE,
    size = 4.5
  ) +
  labs(
    title = "291 WT-abundance Non-orthosteric Variants",
    x = "",
    y = "Activity-abundance residuals",
    fill = ""
  ) +
  theme_classic() +
  theme(
    legend.position = "none"
  ) +
  geom_signif(
    comparisons = list(c("gnomAD", "Pathogenic")),
    map_signif_level = FALSE,
    test = "wilcox.test",
    step_increase = 0.1, y_position = 3.5,
    textsize = 3
  ) + ylim(-5, 5)

```

```
p17 <- plot_grid(p13,p14,p15,p16,ncol=4,nrow=1)
p17
```

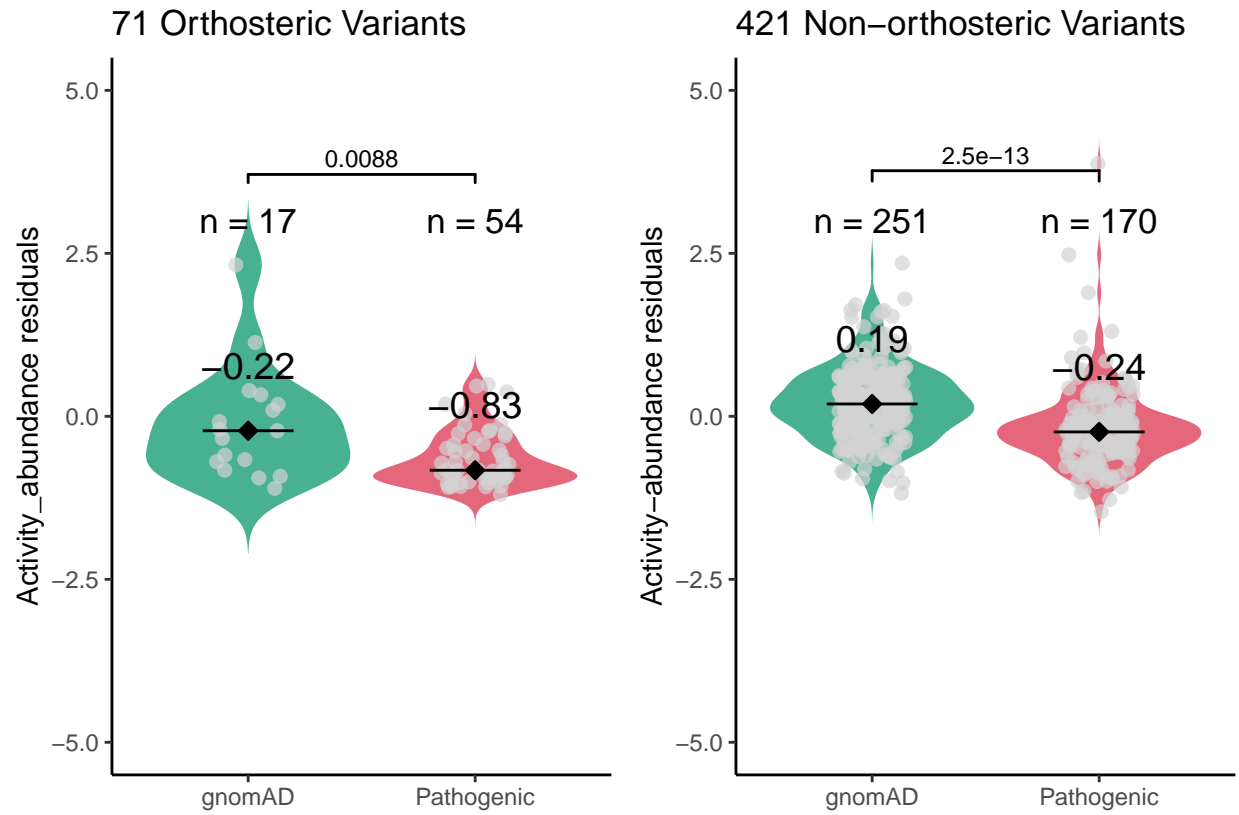


```
p18 <- plot_grid(p13,p14,ncol=2,nrow=1)
p19 <- plot_grid(p15,p16,ncol=2,nrow=1)

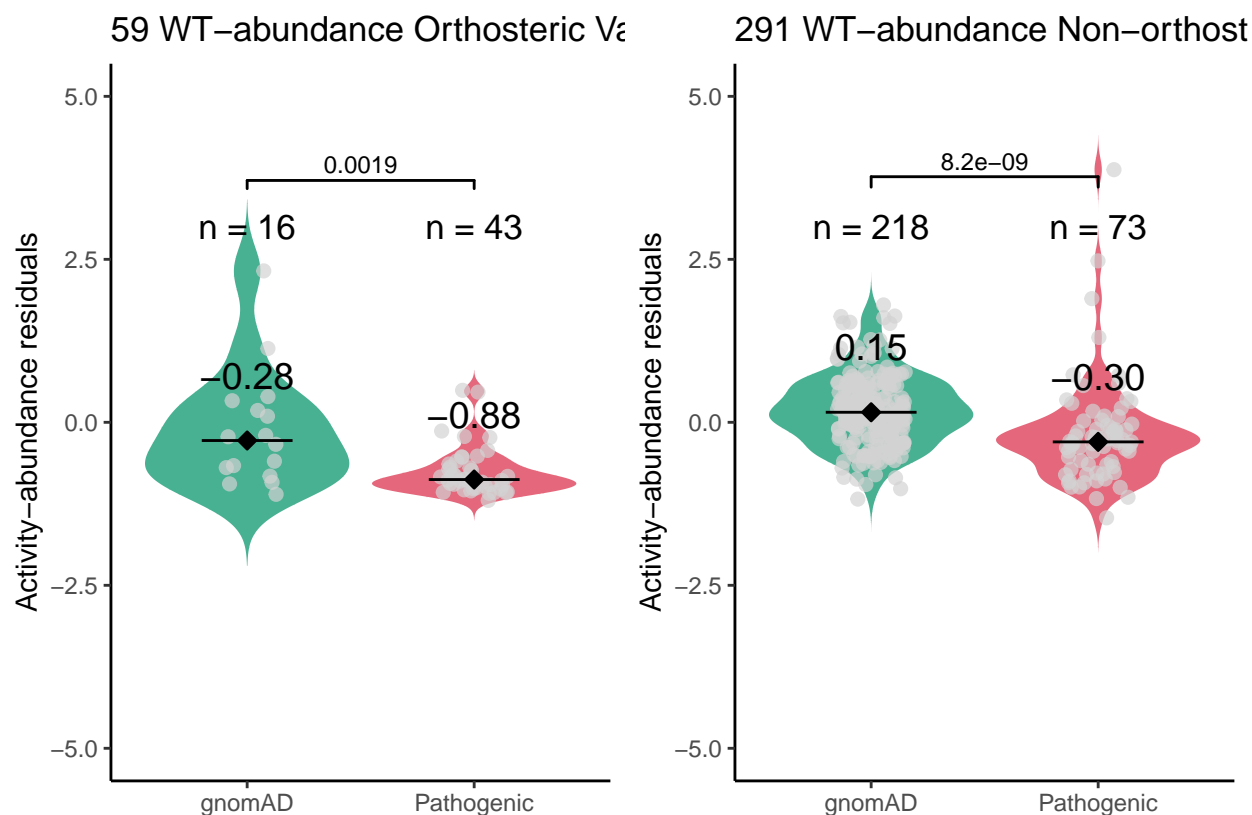
ggsave("/Users/xl7/Documents/01.protein-seq-evo-v1/figs/panels/fig5_violin3.pdf",
  plot = p18, width = 5, height = 3, dpi = 300)

ggsave("/Users/xl7/Documents/01.protein-seq-evo-v1/figs/panels/fig5_violin4.pdf",
  plot = p19, width = 5, height = 3, dpi = 300)

p18
```

p19



```

pdb <- read.pdb("~/Documents/0.Projects/01.protein-seq-evo-v1/data/residual_pdb/GCK/1v4s.pdb")
#unique(pdb$atom$resid)
# Extract C-alpha atoms from protein (exclude ligand)
protein_ca <- pdb$atom[pdb$atom$selety == "CA" & pdb$atom$resid != "GLC" & pdb$atom$resid != "MRK" & pdb$atom$resid != "GCK"]

# Extract ligand atoms (TLA residue)
ligand_atoms <- pdb$atom[pdb$atom$resid == "GLC" & pdb$atom$type == "HETATM", ]

# Calculate min distance from each C-alpha to the ligand
protein_ca$min_dist_to_ligand <- apply(protein_ca, 1, function(atom) {
  dists <- sqrt((as.numeric(atom[["x"]]) - as.numeric(ligand_atoms$x))^2 +
    (as.numeric(atom[["y"]]) - as.numeric(ligand_atoms$y))^2 +
    (as.numeric(atom[["z"]]) - as.numeric(ligand_atoms$z))^2)
  return(min(dists))
})

# View summary
#nrow(protein_ca) #448
#summary(protein_ca$min_dist_to_ligand)
#head(protein_ca$min_dist_to_ligand)
#length(protein_ca$min_dist_to_ligand) #448

#nrow(gck_df_merged)
fil_protein_ca <- protein_ca %>% dplyr::select(resid, resno, min_dist_to_ligand)

```

```

active_positions <- c(151:179, # disordered loop
                     151-153, 168-169, 204-206, 225-231, 254-258, 287, 290, # glucose-binding
                     78:85, 151, 169, 205, 225:229, 295:296, 331:333, 336, 410:416 # ATP-binding
)

active_sites <- c(151:179, # disordered loop
                 78:85, 151, 169, 205, 225:229, 295:296, 331:333, 336, 410:416) # ATP-binding

binding_sites <- c(151:153, 168:169, 204:206, 225:231, 254:258, 287, 290) # glucose-binding)

merged_df <- merge(gck_df, fil_protein_ca, by.x="mutation_position", by.y = "resno", all.x = TRUE)
#nrow(merged_df) #8255

merged_df <- merged_df %>% dplyr::select(-sequence)
nrow(merged_df)

```

```
## [1] 8255
```

```

merged_df <- merged_df[!is.na(merged_df$min_dist_to_ligand),]
nrow(merged_df) #7969

```

```
## [1] 7969
```

```

gnomad_df <- merged_df %>% filter(mutant %in% gnomad_df$mutant)
nrow(gnomad_df)

```

```
## [1] 251
```

```

patho_df1 <- merged_df %>% filter(mutant %in% patho_df1$mutant)
nrow(patho_df1)

```

```
## [1] 3
```

```

patho_df2 <- merged_df %>% filter(mutant %in% patho_df2$mutant)
nrow(patho_df2)

```

```
## [1] 57
```

```

patho_df3 <- merged_df %>% filter(mutant %in% patho_df3$mutant)
nrow(patho_df3)

```

```
## [1] 164
```

```

gnomad_df <- gnomad_df %>% dplyr::select(mutant, DMS_score_abundance, DMS_score_activity, residuals, min
patho_df1 <- patho_df1 %>% dplyr::select(mutant, DMS_score_abundance, DMS_score_activity, residuals, min
patho_df2 <- patho_df2 %>% dplyr::select(mutant, DMS_score_abundance, DMS_score_activity, residuals, min
patho_df3 <- patho_df3 %>% dplyr::select(mutant, DMS_score_abundance, DMS_score_activity, residuals, min

```

```

patho_df1$var_class2 <- "HH"
patho_df2$var_class2 <- "MODY"
patho_df3$var_class2 <- "Monogenic diabetes"
gnomad_df$var_class2 <- "gnomAD"

combined_df <- rbind(patho_df1,patho_df2,patho_df3,gnomad_df)
median_df <- combined_df %>%
  group_by(var_class2) %>%
  summarise(
    median_dist = median(min_dist_to_ligand),
    n = n()
  )
median_df

```

```

## # A tibble: 4 x 3
##   var_class2      median_dist      n
##   <chr>          <dbl> <int>
## 1 HH              16.6      3
## 2 MODY             16.6     57
## 3 Monogenic diabetes 15.6    164
## 4 gnomAD           21.4    251

```

```

combined_df$var_class2 <- factor(
  combined_df$var_class2,
  levels = c("gnomAD", "HH", "MODY", "Monogenic diabetes")
)

custom_colors <- c(
  "gnomAD" = "#1b9e77", # Teal green
  "HH" = "#f4a6b3", # Warm orange
  "MODY" = "#e7298a", # Muted purple
  "Monogenic diabetes" = "#7570b3" # Hot pink / magenta
)

combined_df <- combined_df %>%
  mutate(mutation_position = as.numeric(str_extract(mutant, "(?<=\\D)(\\d+)(?=\\D)")))

combined_df$site_type <- "Non-orthosteric site"
combined_df$site_type[combined_df$mutation_position %in% active_sites] <- "Active site"
combined_df$site_type[combined_df$mutation_position %in% binding_sites] <- "Binding site"
table(combined_df$site_type)

```

```

##
##           Active site           Binding site Non-orthosteric site
##                48                26                401

```

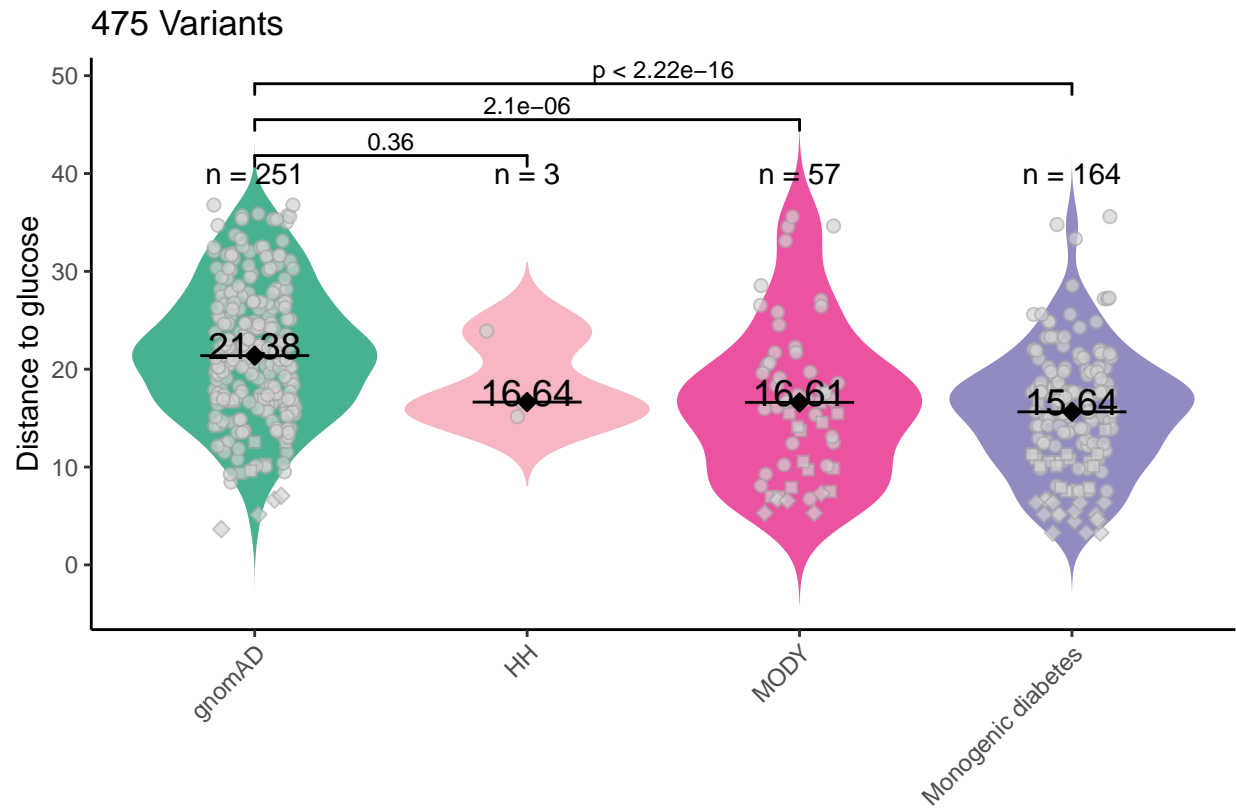
```
nrow(combined_df)
```

```
## [1] 475
```

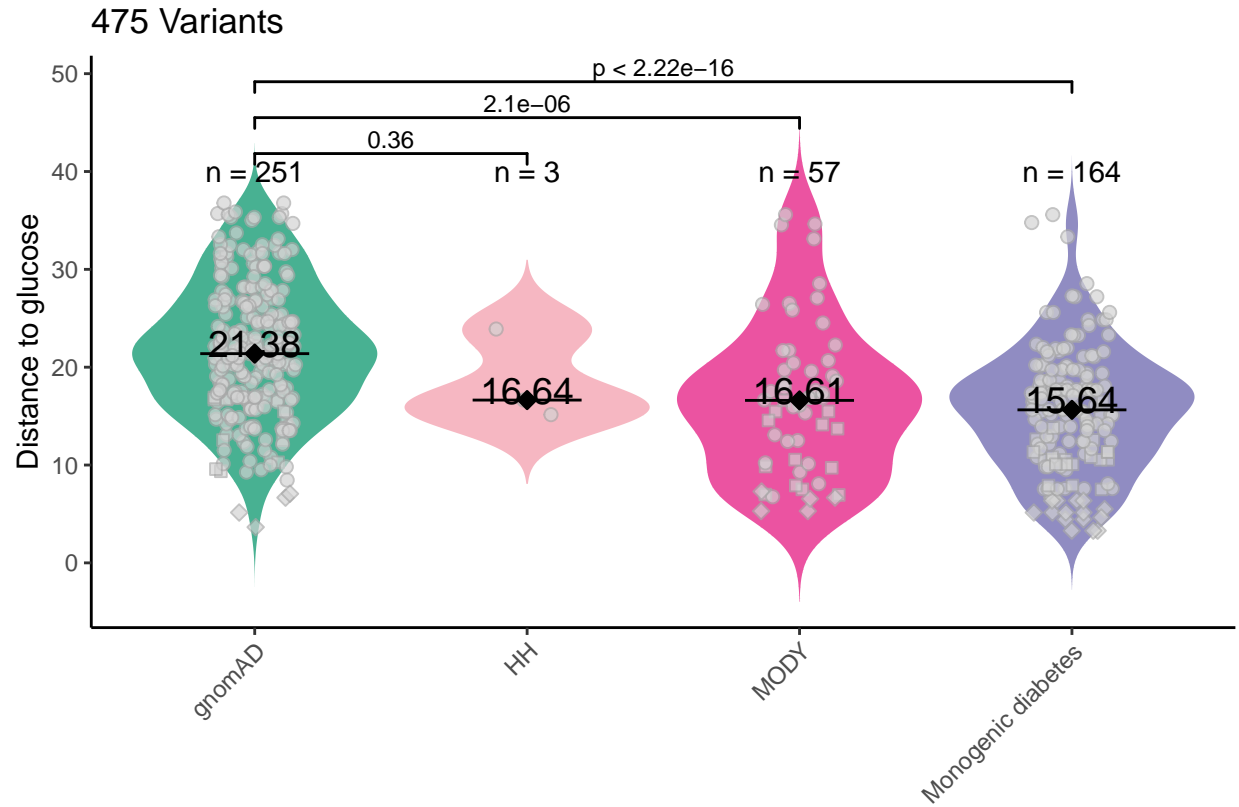
```

p1 <- ggplot(combined_df, aes(x = var_class2, y = min_dist_to_ligand, fill = var_class2)) +
  geom_violin(trim = FALSE, scale = "width", alpha = 0.8, color = NA) +
  geom_jitter(aes(shape = site_type), width = 0.15, size = 2, alpha = 0.7,
    fill = "lightgrey", color = "darkgrey", stroke = 0.5)+
  stat_summary(fun = median, geom = "crossbar", width = 0.4, color = "black", fatten = 1) +
  stat_summary(fun = median, geom = "point", shape = 23, size = 2, fill = "black", color = "black", stroke = 0.5) +
  geom_text(
    data = median_df,
    aes(x = var_class2, y = median_dist + 1, label = sprintf("%.2f", median_dist)),
    inherit.aes = FALSE,
    size = 5
  ) +
  scale_fill_manual(values = custom_colors, guide = "none") +
  scale_shape_manual(values = c(
    "Non-orthosteric site" = 21,
    "Active site" = 22,
    "Binding site" = 23
  )) +
  geom_text(
    data = median_df,
    aes(x = var_class2, y = 40, label = paste0("n = ", n)),
    inherit.aes = FALSE,
    size = 4
  ) +
  labs(
    title = "475 Variants",
    x = "",
    y = "Distance to glucose",
    fill = "",
    shape = "Site Type"
  ) +
  theme_classic() +
  theme(
    legend.position = "none",
    axis.text.x = element_text(angle = 45, hjust = 1)
  ) +
  geom_signif(
    comparisons = list(c("gnomAD", "HH"),
      c("gnomAD", "MODY"),
      c("gnomAD", "Monogenic diabetes")),
    map_signif_level = FALSE,
    test = "wilcox.test",
    step_increase = 0.1,
    textsize = 3
  )
p1

```



```
ggsave("/Users/xl7/Documents/0.Projects/01.protein-seq-evo-v1/figs/panels/fig5_violin5.pdf",
  plot = p1, width = 3, height = 4, dpi = 300)
p1
```

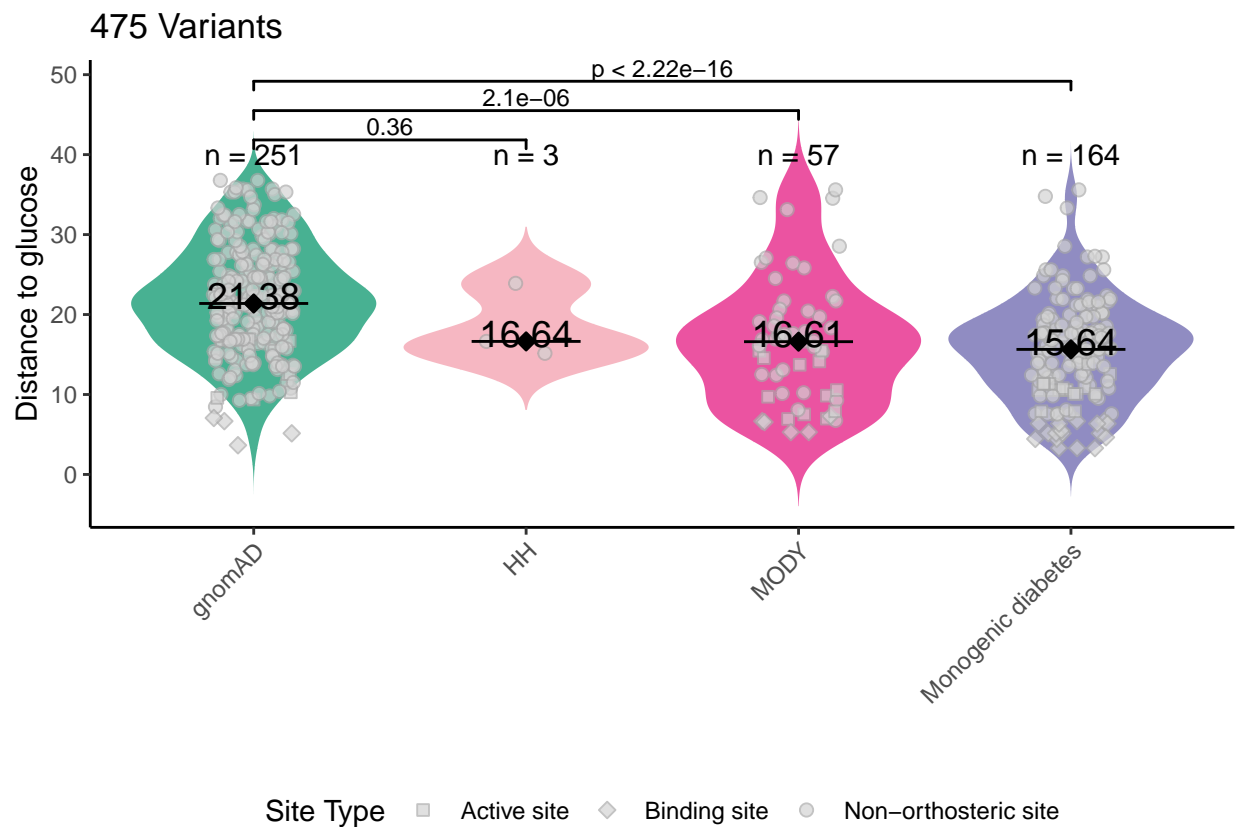


```
ggplot(combined_df, aes(x = var_class2, y = min_dist_to_ligand, fill = var_class2)) +
  geom_violin(trim = FALSE, scale = "width", alpha = 0.8, color = NA) +
  geom_jitter(aes(shape = site_type), width = 0.15, size = 2, alpha = 0.7,
    fill = "lightgrey", color = "darkgrey", stroke = 0.5) +
  stat_summary(fun = median, geom = "crossbar", width = 0.4, color = "black", fatten = 1) +
  stat_summary(fun = median, geom = "point", shape = 23, size = 2, fill = "black", color = "black", stroke = 0.5) +
  geom_text(
    data = median_df,
    aes(x = var_class2, y = median_dist + 1, label = sprintf("%.2f", median_dist)),
    inherit.aes = FALSE,
    size = 5
  ) +
  scale_fill_manual(values = custom_colors, guide = "none") +
  scale_shape_manual(values = c(
    "Non-orthosteric site" = 21,
    "Active site" = 22,
    "Binding site" = 23
  )) +
  geom_text(
    data = median_df,
    aes(x = var_class2, y = 40, label = paste0("n = ", n)),
    inherit.aes = FALSE,
    size = 4
  ) +
  labs(
    title = "475 Variants",
```

```

x = "",
y = "Distance to glucose",
fill = "",
shape = "Site Type"
) +
theme_classic() +
theme(
  legend.position = "bottom",
  axis.text.x = element_text(angle = 45, hjust = 1)
) +
geom_signif(
  comparisons = list(c("gnomAD", "HH"),
                     c("gnomAD", "MODY"),
                     c("gnomAD", "Monogenic diabetes")),
  map_signif_level = FALSE,
  test = "wilcox.test",
  step_increase = 0.1,
  textsize = 3
)

```



```
nrow(merged_df) #7969
```

```
## [1] 7969
```



```
merged_df <- merged_df %>% filter(residuals <=0)
nrow(merged_df) #4417
```

```
## [1] 4417
```

```
merged_df_residue <- merged_df %>%
  group_by(mutation_position) %>%
  summarise(
    loess_residual_avg = median(residuals, na.rm = TRUE))

merged_df_residue <- merge(merged_df_residue, protein_ca, by.x="mutation_position", by.y = "resno", all=TRUE)

merged_df_residue <- merged_df_residue[!is.na(merged_df_residue$min_dist_to_ligand), ]
nrow(merged_df_residue) #445
```

```
## [1] 445
```

```
# Fit exponential decay: y = a * exp(-b * x)
exp_model <- nls(abs(loess_residual_avg) ~ a * exp(-b * min_dist_to_ligand),
  data = merged_df_residue,
  start = list(a = 1, b = 0.1))
exp_model
```

```
## Nonlinear regression model
##   model: abs(loess_residual_avg) ~ a * exp(-b * min_dist_to_ligand)
##   data: merged_df_residue
##      a      b
## 0.9493 0.0438
## residual sum-of-squares: 19.54
##
## Number of iterations to convergence: 4
## Achieved convergence tolerance: 8.104e-07
```

```
# Nonlinear regression model
#   model: abs(loess_residual_avg) ~ a * exp(-b * min_dist_to_ligand)
#   data: merged_df_residue
#      a      b
# 0.9493 0.0438
# residual sum-of-squares: 19.54
#
# Number of iterations to convergence: 4
# Achieved convergence tolerance: 8.104e-07
```

```
a <- 0.9493
b <- 0.0438
half_d <- log(2) / b
half_d #15.82528
```

```
## [1] 15.82528
```

```
y_cutoff <- a * exp(- b * half_d)
y_cutoff
```

```
## [1] 0.47465
```

```
x_vals <- seq(min(merged_df_residue$min_dist_to_ligand),
              max(merged_df_residue$min_dist_to_ligand), length.out = 200)

# --- Bootstrapping for confidence intervals ---
set.seed(11)
boot_params <- replicate(1000, {
  samp <- merged_df_residue[sample(nrow(merged_df_residue), replace = TRUE), ]
  fit <- try(nlsLM(abs(loess_residual_avg) ~ a * exp(-b * min_dist_to_ligand),
                  data = samp, start = list(a = 1, b = 0.1)), silent = TRUE)
  if (inherits(fit, "try-error")) c(NA, NA) else coef(fit)
})
boot_params <- t(boot_params)[complete.cases(t(boot_params)), ]

boot_preds <- apply(boot_params, 1, function(p) p[1] * exp(-p[2] * x_vals))

fit_df_residue <- data.frame(
  min_dist_to_ligand = x_vals,
  loess_residual_avg = predict(exp_model, newdata = data.frame(min_dist_to_ligand = x_vals)),
  lower = apply(boot_preds, 1, quantile, probs = 0.025),
  upper = apply(boot_preds, 1, quantile, probs = 0.975)
)
merged_df_residue$site_type <- "Non-orthosteric site"
merged_df_residue$site_type[abs(merged_df_residue$loess_residual_avg) <= y_cutoff] <- "Null"
merged_df_residue$site_type[merged_df_residue$mutation_position %in% active_sites] <- "ATP-binding site"
merged_df_residue$site_type[merged_df_residue$mutation_position %in% binding_sites] <- "Glucose-binding site"

max(merged_df_residue %>% filter (site_type == "Glucose-binding site") %>% pull(min_dist_to_ligand)) #8
```

```
## [1] 8.666125
```

```
table(merged_df_residue$site_type)
```

```
##
##      ATP-binding site Glucose-binding site Non-orthosteric site
##           45           22           105
##      Null
##      273
```

```
nrow(merged_df_residue) #445
```

```
## [1] 445
```

```
# Plot with fitted curve
p23 <- ggplot(merged_df_residue, aes(x = min_dist_to_ligand, y = abs(loess_residual_avg))) +
  # First, plot NULL points separately with alpha = 0.2
```

```

geom_point(data = subset(merged_df_residue, site_type == "Null"),
           aes(color = site_type), size = 1, alpha = 0.2) +
# Then plot the rest
geom_point(data = subset(merged_df_residue, site_type != "Null"),
           aes(color = site_type), size = 1) +
#geom_text_repel(data = subset(merged_df_residue, mutation_position %in% c(123:130)) ,
#               aes(label = mutation_position, color = site_type), vjust = -0.5, size = 3) +
#geom_text_repel(data = subset(merged_df_residue, mutation_position %in% c(1:14)) ,
#               aes(label = mutation_position, color = site_type), vjust = -0.5, size = 3) +
geom_text_repel(data = merged_df_residue %>% filter (abs(loess_residual_avg) >= y_cutoff) ,
               aes(label = mutation_position, color = site_type), vjust = 0.5, size = 3) +
geom_ribbon(data = fit_df_residue,
           aes(x = min_dist_to_ligand, ymin = lower, ymax = upper),
           fill = "grey70", alpha = 0.3, inherit.aes = FALSE) +
geom_line(data = fit_df_residue, aes(x = min_dist_to_ligand, y = abs(loess_residual_avg)),
          inherit.aes = FALSE, color = "black", size = 1) +
scale_color_manual(values = c(
  "Null" = "grey",
  "Non-orthosteric site" = "darkgreen",
  "ATP-binding site" = "cyan",
  "Glucose-binding site" = "orange"
)) +
theme_classic() +
geom_vline(xintercept = 8.666125, linetype = "dashed", color = "slategrey") +
geom_hline(yintercept = y_cutoff, linetype = "dashed", color = "slategrey") +
labs(
  title = "GCK: per-residue allosteric decay",
  subtitle = "445 residues",
  x = "Minimal distance to glucose",
  y = "Median residual",
  color = ""
) + theme(legend.position = "bottom") +
annotate("text", x = Inf, y = Inf,
          hjust = 1, vjust = 1,
          label = "y = a * exp (b * x)\na = 0.9493 \nb = -0.0438",
          size = 4, color = "black", hjust = 0) + theme(legend.position = "none")

```

```

## Warning: Using 'size' aesthetic for lines was deprecated in ggplot2 3.4.0.
## i Please use 'linewidth' instead.
## This warning is displayed once every 8 hours.
## Call 'lifecycle::last_lifecycle_warnings()' to see where this warning was
## generated.

```

```

## Warning: Duplicated aesthetics after name standardisation: hjust

```

```

p23 <- ggMarginal(
  p23,
  type = "density",
  margins = "both",
  groupColour = FALSE,
  groupFill = FALSE,
  size = 10,
  colour = "grey",

```

```

    fill = "lightgrey"
  )
p23

```

```

## Warning: ggrepel: 136 unlabeled data points (too many overlaps). Consider
## increasing max.overlaps

```

```

ggsave("/Users/xl7/Documents/0.Projects/01.protein-seq-evo-v1/figs/panels/fig5_decay1.pdf",
        plot = p23, width = 5, height = 5, dpi = 300)

```

```

## Warning: ggrepel: 136 unlabeled data points (too many overlaps). Consider
## increasing max.overlaps

```

```

p23

```

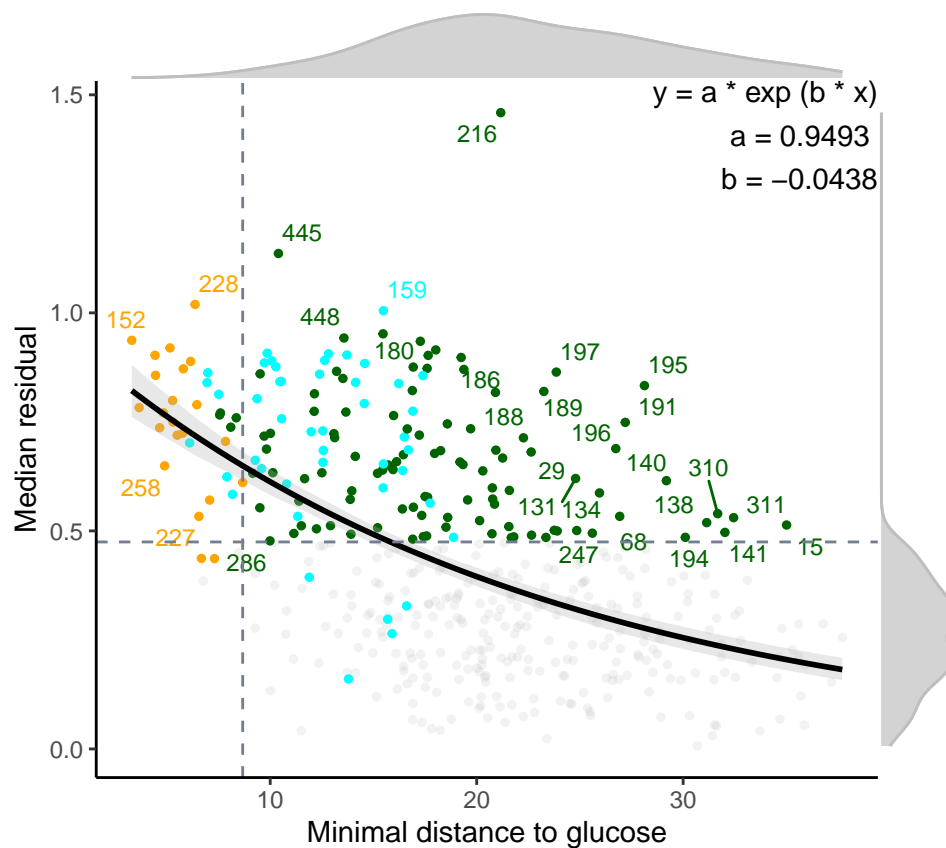
```

## Warning: ggrepel: 136 unlabeled data points (too many overlaps). Consider
## increasing max.overlaps

```

GCK: per-residue allosteric decay

445 residues



```
lm_model <- lm(log(abs(loess_residual_avg)) ~ min_dist_to_ligand, data = merged_df_residue)
summary(lm_model)
```

```
##
## Call:
## lm(formula = log(abs(loess_residual_avg)) ~ min_dist_to_ligand,
##     data = merged_df_residue)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -3.4024 -0.3130  0.1089  0.4467  1.5179
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)   -0.173587   0.085822  -2.023   0.0437 *
## min_dist_to_ligand -0.045660   0.004112 -11.104   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.6397 on 443 degrees of freedom
## Multiple R-squared:  0.2177, Adjusted R-squared:  0.2159
## F-statistic: 123.3 on 1 and 443 DF,  p-value: < 2.2e-16
```

```
# Call:
# lm(formula = log(abs(loess_residual_avg)) ~ min_dist_to_ligand,
#     data = merged_df_residue)
#
# Residuals:
#      Min       1Q   Median       3Q      Max
# -3.4024 -0.3130  0.1089  0.4467  1.5179
#
# Coefficients:
#              Estimate Std. Error t value Pr(>|t|)
# (Intercept)   -0.173587   0.085822  -2.023   0.0437 *
# min_dist_to_ligand -0.045660   0.004112 -11.104   <2e-16 ***
# ---
# Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
#
# Residual standard error: 0.6397 on 443 degrees of freedom
# Multiple R-squared:  0.2177, Adjusted R-squared:  0.2159
# F-statistic: 123.3 on 1 and 443 DF,  p-value: < 2.2e-16
```

```
merged_df$pathogenic_status <- ifelse(
  merged_df$clinvar_clinical_significance %in% c(
    "pathogenic", "likely_pathogenic"),
    "Pathogenic", "Other"
)

nrow(merged_df)
```

```
## [1] 4417
```

```
table(merged_df$pathogenic_status)
```

```
##
##      Other Pathogenic
##      4320          97
```

```
# Fit exponential decay:  $y = a * \exp(-b * x) + c$ 
exp_model <- nls(abs(residuals) ~ a * exp(-b * min_dist_to_ligand),
                 data = merged_df,
                 start = list(a = 1, b = 0.1))
exp_model
```

```
## Nonlinear regression model
##   model: abs(residuals) ~ a * exp(-b * min_dist_to_ligand)
##   data: merged_df
##      a      b
## 0.90290 0.03361
## residual sum-of-squares: 431
##
## Number of iterations to convergence: 4
## Achieved convergence tolerance: 2.906e-07
```

```
# Nonlinear regression model
#   model: abs(residuals) ~ a * exp(-b * min_dist_to_ligand)
#   data: merged_df
#      a      b
# 0.90290 0.03361
# residual sum-of-squares: 431
#
# Number of iterations to convergence: 4
# Achieved convergence tolerance: 2.906e-07
```

```
a <- 0.90290
b <- 0.03361
half_d <- log(2) / b #20.62324
half_d
```

```
## [1] 20.62324
```

```
y_cutoff <- a * exp(-b * half_d)
y_cutoff
```

```
## [1] 0.45145
```

```
merged_df$site_type <- "Non-orthosteric site"
merged_df$site_type[abs(merged_df$residuals) <= y_cutoff] <- "Null"
merged_df$site_type[merged_df$mutation_position %in% active_sites] <- "ATP-binding site"
merged_df$site_type[merged_df$mutation_position %in% binding_sites] <- "Glucose-binding site"

x_vals <- seq(min(merged_df$min_dist_to_ligand, na.rm = TRUE),
```

```

max(merged_df$min_dist_to_ligand, na.rm = TRUE), length.out = 200)

set.seed(11)
boot_params <- replicate(1000, {
  samp <- merged_df[sample(nrow(merged_df), replace = TRUE), ]
  fit <- try(nlsLM(abs(residuals) ~ a * exp(-b * min_dist_to_ligand),
    data = samp, start = list(a = 1, b = 0.1)), silent = TRUE)
  if (inherits(fit, "try-error")) c(NA, NA) else coef(fit)
})
boot_params <- t(boot_params)[complete.cases(t(boot_params)), ]

boot_preds <- apply(boot_params, 1, function(p) p[1] * exp(-p[2] * x_vals))

fit_df_residue <- data.frame(
  min_dist_to_ligand = x_vals,
  residuals = predict(exp_model, newdata = data.frame(min_dist_to_ligand = x_vals)),
  lower = apply(boot_preds, 1, quantile, probs = 0.025),
  upper = apply(boot_preds, 1, quantile, probs = 0.975)
)

# Plot
p24 <- ggplot(merged_df, aes(x = min_dist_to_ligand, y = abs(residuals))) +
  # Base layer: all points
  geom_point(aes(color = site_type, alpha = pathogenic_status, shape = pathogenic_status), size = 2) +
  geom_ribbon(data = fit_df_residue,
    aes(x = min_dist_to_ligand, ymin = lower, ymax = upper),
    fill = "grey70", alpha = 0.3, inherit.aes = FALSE) +
  geom_line(data = fit_df_residue, aes(x = min_dist_to_ligand, y = abs(residuals)),
    inherit.aes = FALSE, color = "black", size = 1) +

  # Repelled text labels for selected mutations
  geom_text_repel(
    data = subset(merged_df, pathogenic_status == "Pathogenic" & min_dist_to_ligand > 8.666125 & site_type != "Null"),
    aes(label = mutant, color = site_type),
    size = 3,
    max.overlaps = Inf, box.padding = 0.4, point.padding = 0.3
  ) +

  # Manual color palette for site type
  scale_color_manual(values = c(
    "Null" = "grey",
    "Non-orthosteric site" = "darkgreen",
    "ATP-binding site" = "cyan",
    "Glucose-binding site" = "orange"
  )) +

  # Transparency scale
  scale_alpha_manual(values = c("Other" = 0.1, "Pathogenic" = 1)) +

  # Reference lines
  geom_vline(xintercept = 8.666125, linetype = "dashed", color = "slategrey") +
  geom_hline(yintercept = y_cutoff, linetype = "dashed", color = "slategrey") +
  theme_classic() +

```

```

labs(
  title = "GCK: per-mutation allosteric decay",
  subtitle = "4417 mutations with residuals >= 0",
  x = "Minimal distance to glucose",
  y = "LOESS residual",
  color = ""
) + theme(legend.position = "bottom") + guides(color = "none", alpha = "none") +
  annotate("text", x = Inf, y = Inf,
    hjust = 1, vjust = 1,
    label = "y = a * exp (b * x)\na = 0.90290 \nb = - 0.03361",
    size = 4, color = "black", hjust = 0) + theme(legend.position = "none")

```

Warning: Duplicated aesthetics after name standardisation: hjust

```

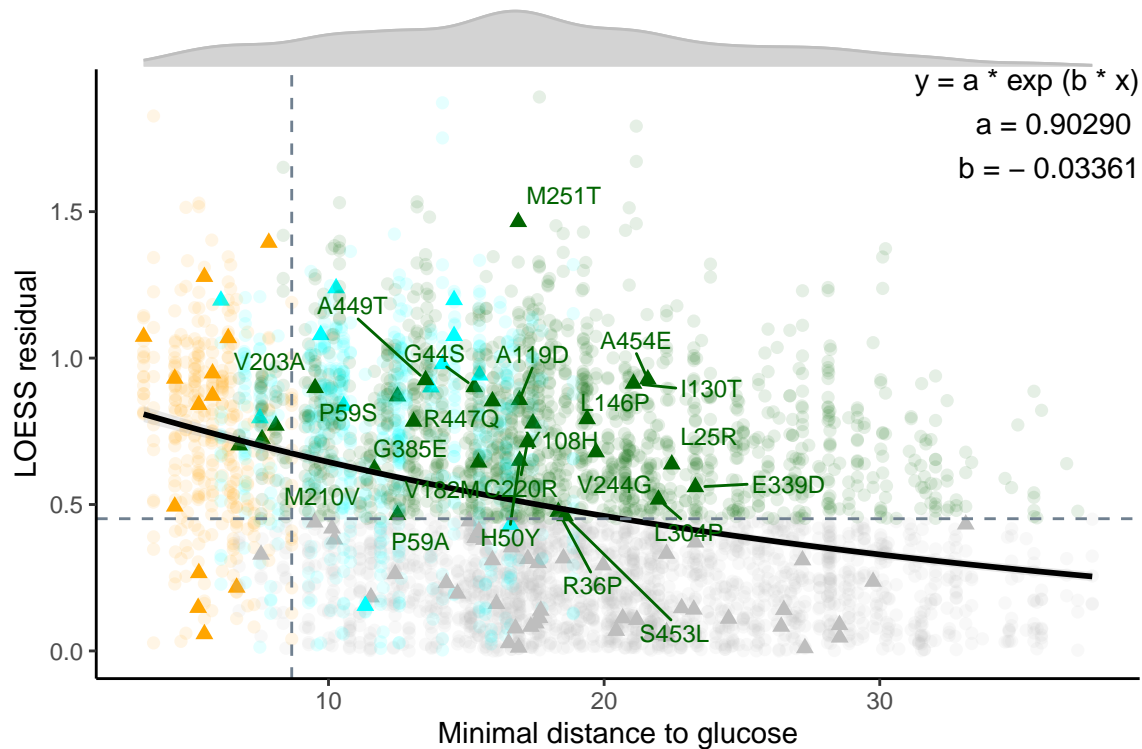
p24 <- ggMarginal(
  p24,
  type = "density",
  margins = "both",
  groupColour = FALSE,
  groupFill = FALSE,
  size = 10,
  colour = "grey",
  fill = "lightgrey"
)
p24

ggsave("/Users/xl7/Documents/0.Projects/01.protein-seq-evo-v1/figs/panels/fig5_decay2.pdf",
  plot = p24, width = 5, height = 5, dpi = 300)
p24

```


GCK: per-mutation allosteric decay

4417 mutations with residuals ≥ 0



```
lm_model <- lm(log(abs(residuals)) ~ min_dist_to_ligand, data = merged_df)
summary(lm_model)
```

```
##
## Call:
## lm(formula = log(abs(residuals)) ~ min_dist_to_ligand, data = merged_df)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -8.7790 -0.4103  0.2504  0.6455  1.8923
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)   -0.233775   0.039517  -5.916 3.55e-09 ***
## min_dist_to_ligand -0.044398   0.002099 -21.154 < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 1.001 on 4415 degrees of freedom
## Multiple R-squared:  0.09203,    Adjusted R-squared:  0.09183
## F-statistic: 447.5 on 1 and 4415 DF,  p-value: < 2.2e-16
```

```
# Call:
# lm(formula = log(abs(residuals)) ~ min_dist_to_ligand, data = merged_df)
#
```

```
# Residuals:
#      Min       1Q   Median       3Q      Max
# -8.7790 -0.4103  0.2504  0.6455  1.8923
#
# Coefficients:
#              Estimate Std. Error t value Pr(>|t|)
# (Intercept)   -0.233775    0.039517  -5.916 3.55e-09 ***
# min_dist_to_ligand -0.044398    0.002099 -21.154 < 2e-16 ***
# ---
# Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
#
# Residual standard error: 1.001 on 4415 degrees of freedom
# Multiple R-squared:  0.09203, Adjusted R-squared:  0.09183
# F-statistic: 447.5 on 1 and 4415 DF,  p-value: < 2.2e-16
```

```
nrow(merged_df) #4417
```

```
## [1] 4417
```

```
merged_df <- merge(gck_df, fil_protein_ca, by.x="mutation_position", by.y = "resno", all.x = TRUE)
#nrow(merged_df) #8255
```

```
merged_df <- merged_df %>% dplyr::select(-sequence)
nrow(merged_df)
```

```
## [1] 8255
```

```
merged_df <- merged_df[!is.na(merged_df$min_dist_to_ligand),]
nrow(merged_df) #7969
```

```
## [1] 7969
```

```
merged_df$pathogenic_status <- ifelse(
  merged_df$clinvar_clinical_significance %in% c(
    "pathogenic", "likely_pathogenic",
    "Pathogenic", "Other"
  )
)

merged_df_int <- merged_df %>% filter(mutation_position %in% active_positions)
nrow(merged_df_int) #1031
```

```
## [1] 1031
```

```
table(merged_df_int$pathogenic_status)
```

```
##
##      Other Pathogenic
##      1009          22
```

```
# Other Pathogenic
#      1009      22

merged_df_out <- merged_df %>% filter(!mutation_position %in% active_positions)
nrow(merged_df_out) #6938
```

```
## [1] 6938
```

```
table(merged_df_out$pathogenic_status)
```

```
##
##      Other Pathogenic
##      6829      109
```

```
# Other Pathogenic
# 6829      109
```

```
# 1. Set up
set.seed(123)
n_boot <- 1000
match_window <- 0.05
n_patho <- nrow(merged_df_int %>% filter(pathogenic_status == "Pathogenic"))

# 2. Get abundance/residuals from pten_patho
patho_df <- merged_df_int %>% filter(pathogenic_status == "Pathogenic") %>% dplyr::select(DMS_score_abun
patho_df$group <- "Pathogenic"

# 3. Bootstrap sampling from non-patho pool with abundance matching
non_patho_pool <- merged_df_int %>% filter(pathogenic_status != "Pathogenic") %>%
  filter(!(mutant %in% patho_df$mutant))

bootstrap_medians <- vector("numeric", length = n_boot)

# Pre-group non-patho pool into bins
non_patho_pool <- non_patho_pool %>%
  mutate(bin = cut(DMS_score_abundance, breaks = seq(-0.5, 2, by = match_window)))

# Bin pathogenic variants accordingly
patho_df <- patho_df %>%
  mutate(bin = cut(DMS_score_abundance, breaks = seq(-0.5, 2, by = match_window)))

# Create lookup table for fast sampling
bin_lookup <- split(non_patho_pool$residuals, non_patho_pool$bin)

# Bootstrap matrix
bootstrap_matrix <- matrix(NA, nrow = n_boot, ncol = n_patho)

for (i in 1:n_boot) {
  for (j in 1:n_patho) {
    bin_j <- patho_df$bin[j]
    candidates <- bin_lookup[[as.character(bin_j)]]
    if (!is.null(candidates) && length(candidates) > 0) {
```

```

    bootstrap_matrix[i, j] <- sample(candidates, 1)
  }
}
}

# Summarize into a dataframe
boot_df <- data.frame(
  group = "Random abundance-matched",
  residuals = apply(bootstrap_matrix, 1, median, na.rm = TRUE) # Mean across matches per bootstrap
)

# Combine with patho residuals
plot_df <- bind_rows(
  patho_df %>% dplyr::select(group, residuals),
  boot_df
)

label_df <- plot_df %>%
  group_by(group) %>%
  summarise(
    n = n(),
    median_val = median(residuals),
    y_max = max(residuals),
    .groups = "drop"
  )

label_df <- label_df %>%
  mutate(n_label = case_when(
    group == "Random abundance-matched" ~ "bootstrapped 1000 times",
    TRUE ~ paste0("n = ", n)
  ))

# Plot
p_fast <- ggplot(plot_df, aes(x = group, y = residuals, fill = group)) +
  geom_violin(trim = FALSE, scale = "width", alpha = 0.8, color = NA) +
  geom_jitter(width = 0.15, size = 2, alpha = 0.7, color = "lightgrey") +
  stat_summary(fun = median, geom = "crossbar", width = 0.4, color = "black", fatten = 1) +
  stat_summary(fun = median, geom = "point", shape = 23, size = 2.5,
    fill = "black", color = "black", stroke = 0.7) +

  geom_text(
    data = label_df,
    aes(x = group, y = 2.5, label = n_label),
    inherit.aes = FALSE,
    size = 4) +

  geom_text(
    data = label_df,
    aes(x = group, y = median_val + 0.25, label = sprintf(" %.2f", median_val)),
    inherit.aes = FALSE,
    size = 6
  ) +
  labs(

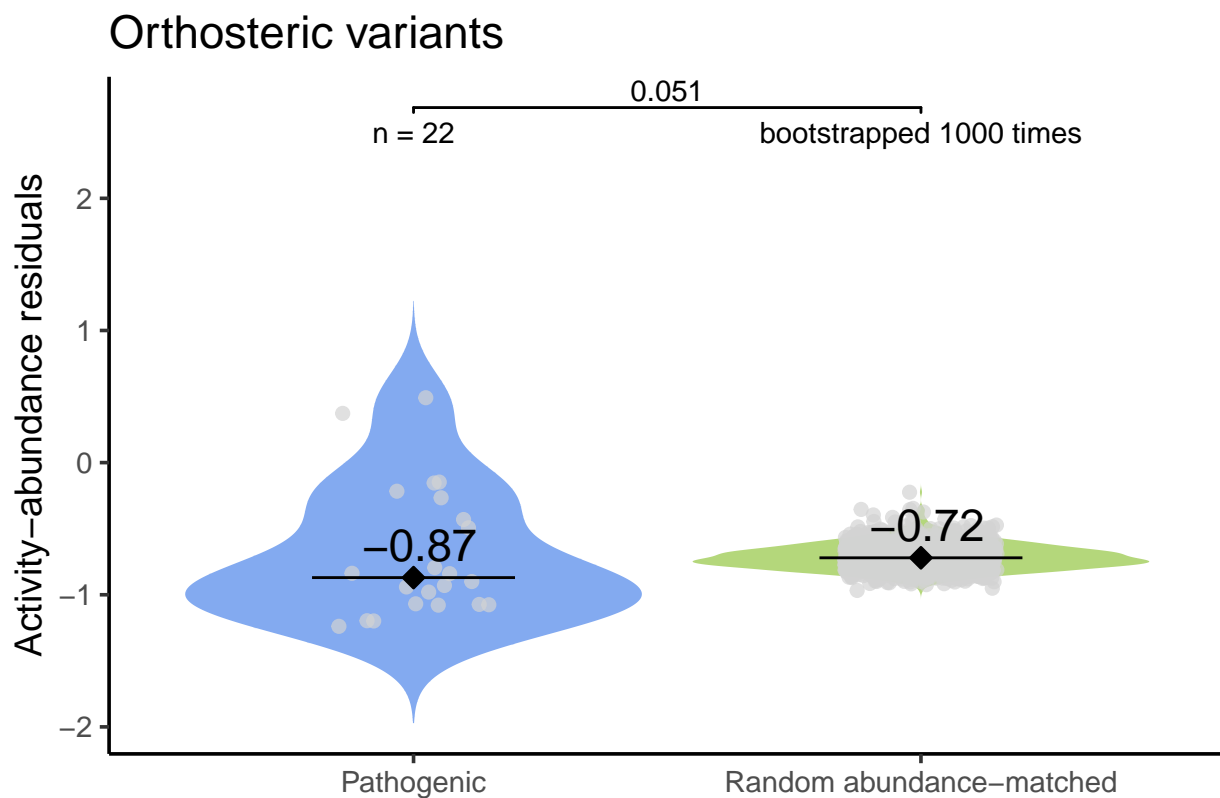
```

```

x = "",
y = "Activity-abundance residuals",
title = "Orthosteric variants"
) +
theme_classic(base_size = 14) +
scale_fill_manual(values = c("Pathogenic" = "cornflowerblue", "Random abundance-matched" = "darkolivegreen3"))
theme(legend.position = "none") +
geom_signif(comparisons = list(c("Pathogenic", "Random abundance-matched")),
            map_signif_level = FALSE,
            test = "wilcox.test",
            tip_length = 0.01)

```

p_fast



merged_df_out

##	mutation_position	mutant	DMS_score_abundance	DMS_score_bin_abundance
## 1	14	E14F	0.9236349927	1
## 2	14	E14K	0.6822279598	1
## 3	14	E14N	1.0989437191	1
## 4	14	E14D	1.0347078815	1
## 5	14	E14R	0.6415446254	1
## 6	14	E14G	1.0734105136	1
## 7	14	E14L	0.8292057551	1
## 8	14	E14C	1.0771280792	1

## 9	14	E14M	1.1829704101	1
## 10	14	E14I	0.6621624585	1
## 11	14	E14S	1.0319348748	1
## 12	14	E14Q	1.3925578790	1
## 13	14	E14H	0.3765360307	0
## 14	14	E14Y	0.9683740774	1
## 15	14	E14T	0.7805120023	1
## 16	14	E14P	0.8538277389	1
## 17	14	E14A	0.6448758289	1
## 18	14	E14W	0.5660312265	0
## 19	14	E14V	0.9874310358	1
## 20	15	K15A	1.1965444818	1
## 21	15	K15W	0.7959186366	1
## 22	15	K15Y	0.8323110172	1
## 23	15	K15V	0.8142525060	1
## 24	15	K15Q	0.8933471165	1
## 25	15	K15C	0.6046316890	1
## 26	15	K15S	1.1286506216	1
## 27	15	K15T	1.1644461990	1
## 28	15	K15M	1.0386946022	1
## 29	15	K15E	0.5804396704	0
## 30	15	K15G	1.0980083255	1
## 31	15	K15D	0.8315379870	1
## 32	15	K15I	1.1517931035	1
## 33	15	K15P	0.9014119175	1
## 34	15	K15F	0.8221903280	1
## 35	15	K15R	0.8897428652	1
## 36	15	K15L	1.0217651425	1
## 37	15	K15H	0.5327446470	0
## 38	16	V16A	0.6210932698	1
## 39	16	V16D	0.4289736660	0
## 40	16	V16E	1.0815769841	1
## 41	16	V16F	1.1876969707	1
## 42	16	V16G	0.5976289320	0
## 43	16	V16H	0.8319247386	1
## 44	16	V16I	0.9278690184	1
## 45	16	V16K	-0.0003922806	0
## 46	16	V16L	1.1680980082	1
## 47	16	V16M	1.0148417287	1
## 48	16	V16N	0.2870340298	0
## 49	16	V16P	0.3963190798	0
## 50	16	V16Q	0.4640327667	0
## 51	16	V16R	0.5955258386	0
## 52	16	V16S	1.0581265369	1
## 53	16	V16T	0.3701878225	0
## 54	16	V16W	1.2425861289	1
## 55	16	V16Y	0.7973123905	1
## 56	17	E17P	0.3299966750	0
## 57	17	E17Q	1.0801916063	1
## 58	17	E17H	0.7661149584	1
## 59	17	E17G	0.6392790863	1
## 60	17	E17Y	1.0042569966	1
## 61	17	E17L	0.6046876388	1
## 62	17	E17N	0.8730747314	1

## 63	17	E17I	1.1200789420	1
## 64	17	E17K	0.5185825870	0
## 65	17	E17F	1.0748030457	1
## 66	17	E17S	1.0515267071	1
## 67	17	E17R	0.7110945928	1
## 68	17	E17T	0.9251516071	1
## 69	17	E17W	0.5899384078	0
## 70	17	E17D	0.5183389584	0
## 71	17	E17A	0.7506776684	1
## 72	17	E17V	0.7883167021	1
## 73	17	E17C	0.7173415206	1
## 74	18	Q18E	1.0279758814	1
## 75	18	Q18C	1.1611151641	1
## 76	18	Q18D	1.3225362379	1
## 77	18	Q18V	0.7893041862	1
## 78	18	Q18Y	0.5265404515	0
## 79	18	Q18N	0.9106941818	1
## 80	18	Q18G	0.7869125773	1
## 81	18	Q18H	1.2555568245	1
## 82	18	Q18W	1.1421114939	1
## 83	18	Q18T	0.7330882239	1
## 84	18	Q18M	0.5972687075	0
## 85	18	Q18P	0.7655736178	1
## 86	18	Q18R	0.6639227322	1
## 87	18	Q18F	1.1280816377	1
## 88	18	Q18A	0.9690977369	1
## 89	18	Q18L	0.7535629272	1
## 90	18	Q18S	1.1996920356	1
## 91	18	Q18K	1.0810958478	1
## 92	18	Q18I	1.2538557744	1
## 93	19	I19T	1.0820752227	1
## 94	19	I19S	0.5835425162	0
## 95	19	I19C	1.0586603123	1
## 96	19	I19V	1.0685687752	1
## 97	19	I19N	0.6926638599	1
## 98	19	I19A	0.4965283001	0
## 99	19	I19W	1.1529157080	1
## 100	19	I19R	0.9944254811	1
## 101	19	I19E	0.7857949908	1
## 102	19	I19L	0.8256016859	1
## 103	19	I19Q	0.2900708801	0
## 104	19	I19D	0.4707338433	0
## 105	19	I19H	0.7130502547	1
## 106	19	I19F	0.9696194194	1
## 107	19	I19K	0.3908447575	0
## 108	19	I19M	0.8849645793	1
## 109	19	I19Y	0.2729254559	0
## 110	19	I19G	0.1949459373	0
## 111	20	L20F	0.7654301678	1
## 112	20	L20T	1.2174513022	1
## 113	20	L20W	1.1718692731	1
## 114	20	L20I	-0.2551072053	0
## 115	20	L20G	0.0028592783	0
## 116	20	L20E	0.3462148834	0

## 117	20	L20H	-0.1416799008	0
## 118	20	L20S	-0.0579779884	0
## 119	20	L20K	-0.1626267317	0
## 120	20	L20D	0.0759123870	0
## 121	20	L20N	-0.3069291231	0
## 122	20	L20C	1.1134362176	1
## 123	20	L20R	-0.1335371530	0
## 124	20	L20A	-0.3107381046	0
## 125	20	L20V	0.6957508011	1
## 126	20	L20Q	-0.3605344429	0
## 127	20	L20M	0.7938868448	1
## 128	20	L20Y	0.8854244257	1
## 129	20	L20P	0.0917206362	0
## 130	21	A21L	0.6737779823	1
## 131	21	A21K	0.7542903169	1
## 132	21	A21E	1.0864687490	1
## 133	21	A21P	-0.1687609031	0
## 134	21	A21I	-0.1221221988	0
## 135	21	A21G	1.1353821760	1
## 136	21	A21D	1.2351496263	1
## 137	21	A21C	1.0901603756	1
## 138	21	A21M	0.8210251997	1
## 139	21	A21H	1.2427829100	1
## 140	21	A21R	0.7855550460	1
## 141	21	A21V	1.1187143953	1
## 142	21	A21Q	0.0454365268	0
## 143	21	A21Y	1.2744607895	1
## 144	21	A21W	1.1885714365	1
## 145	21	A21N	-0.0595606850	0
## 146	21	A21S	0.7501195770	1
## 147	21	A21T	0.6816068195	1
## 148	22	E22D	1.1873858740	1
## 149	22	E22A	0.7550065093	1
## 150	22	E22Y	0.7764528729	1
## 151	22	E22W	0.8831022044	1
## 152	22	E22L	0.6177565091	1
## 153	22	E22H	1.0319031104	1
## 154	22	E22C	0.6079502531	1
## 155	22	E22G	0.5411222659	0
## 156	22	E22F	0.3743940616	0
## 157	22	E22M	0.5639791376	0
## 158	22	E22K	0.8368429983	1
## 159	22	E22T	0.7322588225	1
## 160	22	E22R	0.9151455894	1
## 161	22	E22N	0.8681833818	1
## 162	22	E22V	0.8737800336	1
## 163	22	E22S	0.5652386881	0
## 164	22	E22Q	0.3459741060	0
## 165	22	E22I	0.9549754027	1
## 166	23	F23W	0.7136527796	1
## 167	23	F23L	0.8303010796	1
## 168	23	F23V	0.0716815921	0
## 169	23	F23H	-0.0174725017	0
## 170	23	F23G	0.1697170565	0

## 171	23	F23M	0.6844953821	1
## 172	23	F23K	0.1853563749	0
## 173	23	F23N	-0.1198252649	0
## 174	23	F23D	0.0452473274	0
## 175	23	F23S	-0.7397996541	0
## 176	23	F23T	-0.0400394092	0
## 177	23	F23A	0.6237149683	1
## 178	23	F23C	0.3295003938	0
## 179	23	F23R	-0.1736240714	0
## 180	23	F23Q	-0.2782817411	0
## 181	23	F23P	-0.3376980369	0
## 182	24	Q24F	0.7619780542	1
## 183	24	Q24E	1.0417271830	1
## 184	24	Q24L	0.5964252636	0
## 185	24	Q24G	1.0341449540	1
## 186	24	Q24I	0.9572013965	1
## 187	24	Q24K	1.2430694408	1
## 188	24	Q24Y	0.5043665165	0
## 189	24	Q24C	1.1568730687	1
## 190	24	Q24M	0.6034885587	1
## 191	24	Q24W	1.6096086820	1
## 192	24	Q24A	0.9118139543	1
## 193	24	Q24R	1.0818180764	1
## 194	24	Q24S	0.8996824478	1
## 195	24	Q24T	0.7575061169	1
## 196	24	Q24P	0.3684823068	0
## 197	24	Q24V	1.0773401203	1
## 198	25	L25N	0.3815380704	0
## 199	25	L25P	0.6436657924	1
## 200	25	L25D	0.3434327575	0
## 201	25	L25G	0.3618481365	0
## 202	25	L25F	0.7040445414	1
## 203	25	L25M	0.7786772565	1
## 204	25	L25Q	0.6033910018	1
## 205	25	L25E	-0.1317515427	0
## 206	25	L25I	0.7926765646	1
## 207	25	L25R	0.1731616409	0
## 208	25	L25S	0.5771965740	0
## 209	25	L25T	0.5339511844	0
## 210	25	L25C	0.7091217295	1
## 211	25	L25W	1.0576611437	1
## 212	25	L25Y	0.7937442117	1
## 213	25	L25H	0.5167175622	0
## 214	25	L25V	0.7479324339	1
## 215	25	L25K	0.4714927930	0
## 216	25	L25A	0.7449972334	1
## 217	26	Q26A	0.7085133008	1
## 218	26	Q26C	1.1844240731	1
## 219	26	Q26D	0.8130448027	1
## 220	26	Q26F	0.8416029291	1
## 221	26	Q26M	0.4263349304	0
## 222	26	Q26N	1.1739656434	1
## 223	26	Q26E	1.0449078049	1
## 224	26	Q26R	0.6626509155	1

## 225	26	Q26S	0.9288512157	1
## 226	26	Q26T	1.0948111768	1
## 227	26	Q26P	0.6732365390	1
## 228	26	Q26K	0.5791674926	0
## 229	26	Q26L	0.7448369205	1
## 230	26	Q26G	0.8921090660	1
## 231	26	Q26Y	0.4708631269	0
## 232	26	Q26V	0.9791815379	1
## 233	26	Q26W	0.7481492920	1
## 234	26	Q26I	0.8665781773	1
## 235	27	E27K	1.0225066945	1
## 236	27	E27F	0.2806254740	0
## 237	27	E27S	0.4986702378	0
## 238	27	E27L	0.9662841219	1
## 239	27	E27N	0.3222826596	0
## 240	27	E27R	0.2548686945	0
## 241	27	E27I	0.5278632201	0
## 242	27	E27Y	0.7784756652	1
## 243	27	E27C	0.3461721447	0
## 244	27	E27V	0.6294296369	1
## 245	27	E27T	0.6343976769	1
## 246	27	E27W	0.5891066095	0
## 247	27	E27A	1.1549575788	1
## 248	27	E27P	0.2239934409	0
## 249	27	E27M	0.3886361914	0
## 250	27	E27G	0.7153293556	1
## 251	27	E27Q	0.6191894605	1
## 252	27	E27H	1.1163908561	1
## 253	28	E28Q	0.6390626806	1
## 254	28	E28P	0.4783515780	0
## 255	28	E28V	0.5967475905	0
## 256	28	E28A	0.7999790765	1
## 257	28	E28N	0.4014699260	0
## 258	28	E28K	0.8973969571	1
## 259	28	E28I	0.8027321442	1
## 260	28	E28S	0.9657951832	1
## 261	28	E28W	0.7714217632	1
## 262	28	E28M	1.0953034787	1
## 263	28	E28T	0.3185674434	0
## 264	28	E28H	1.2275915777	1
## 265	28	E28G	0.9098556323	1
## 266	28	E28C	0.5445234274	0
## 267	28	E28L	0.6373243546	1
## 268	28	E28F	1.2485441371	1
## 269	28	E28D	0.8077692476	1
## 270	28	E28R	0.6370513816	1
## 271	28	E28Y	0.6059230942	1
## 272	29	D29S	0.9297662717	1
## 273	29	D29Q	0.9314260177	1
## 274	29	D29C	0.8299971843	1
## 275	29	D29R	0.5886817857	0
## 276	29	D29L	0.6340446513	1
## 277	29	D29V	0.9458923622	1
## 278	29	D29T	0.4876286029	0

## 279	29	D29E	0.4805544090	0
## 280	29	D29K	0.6304898034	1
## 281	29	D29I	0.0160319097	0
## 282	29	D29A	1.2533344454	1
## 283	29	D29P	0.0969741628	0
## 284	29	D29M	0.3199358006	0
## 285	29	D29F	0.7778452688	1
## 286	29	D29W	0.2748572724	0
## 287	29	D29G	0.3976269327	0
## 288	30	L30R	0.9752425566	1
## 289	30	L30Q	1.1371747572	1
## 290	30	L30C	0.9945089298	1
## 291	30	L30P	-0.0404831609	0
## 292	30	L30A	1.0804349808	1
## 293	30	L30G	0.0140841590	0
## 294	30	L30S	0.8550887124	1
## 295	30	L30N	0.2789432866	0
## 296	30	L30Y	0.4809522347	0
## 297	30	L30E	0.9284640094	1
## 298	30	L30T	1.0297250366	1
## 299	30	L30D	0.6386044304	1
## 300	30	L30F	-0.2723322027	0
## 301	30	L30K	0.4793612675	0
## 302	30	L30W	0.3689373283	0
## 303	30	L30H	0.6429806557	1
## 304	30	L30V	0.9495535073	1
## 305	30	L30I	1.1489415496	1
## 306	31	K31Y	0.5045601556	0
## 307	31	K31W	0.7100241838	1
## 308	31	K31T	0.3380660758	0
## 309	31	K31A	0.7194447846	1
## 310	31	K31V	0.7101042616	1
## 311	31	K31S	0.8099990009	1
## 312	31	K31D	1.1584113174	1
## 313	31	K31N	0.5035380954	0
## 314	31	K31F	0.9053289010	1
## 315	31	K31C	0.6601555924	1
## 316	31	K31P	0.3928649541	0
## 317	31	K31I	1.2599278604	1
## 318	31	K31E	1.1437176474	1
## 319	31	K31R	0.9061418122	1
## 320	31	K31Q	0.8643546901	1
## 321	31	K31L	0.7367705202	1
## 322	31	K31G	0.7726363601	1
## 323	31	K31H	0.4202905367	0
## 324	32	K32S	0.8200243141	1
## 325	32	K32R	0.7478352115	1
## 326	32	K32T	0.7654749710	1
## 327	32	K32G	0.8938553354	1
## 328	32	K32A	0.7130814275	1
## 329	32	K32C	1.1396360542	1
## 330	32	K32V	0.8612529424	1
## 331	32	K32D	0.9890765022	1
## 332	32	K32H	0.6465547044	1

## 333	32	K32I	0.9033019504	1
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## 335	32	K32Q	0.9186892622	1
## 336	32	K32E	0.8741284805	1
## 337	32	K32F	0.7656125535	1
## 338	32	K32W	0.8396614187	1
## 339	32	K32L	0.8999326127	1
## 340	32	K32M	0.6940754083	1
## 341	32	K32P	0.0457058508	0
## 342	33	V33A	0.8002033662	1
## 343	33	V33C	0.8663483907	1
## 344	33	V33E	0.0806269616	0
## 345	33	V33F	0.6545445182	1
## 346	33	V33G	0.0299600519	0
## 347	33	V33H	0.6262314894	1
## 348	33	V33I	0.9910193421	1
## 349	33	V33K	-0.5052331740	0
## 350	33	V33L	0.7701435250	1
## 351	33	V33M	0.3658217401	0
## 352	33	V33N	-0.4610740867	0
## 353	33	V33P	0.4456435183	0
## 354	33	V33Q	0.3538751702	0
## 355	33	V33R	-0.3468896264	0
## 356	33	V33S	0.1161785805	0
## 357	33	V33T	0.9501387138	1
## 358	33	V33W	0.4204815957	0
## 359	33	V33Y	-0.2409849441	0
## 360	34	M34P	-0.2663570911	0
## 361	34	M34N	-0.1954665056	0
## 362	34	M34E	0.4372812106	0
## 363	34	M34H	0.5100344135	0
## 364	34	M34L	0.7117453879	1
## 365	34	M34C	0.6493191405	1
## 366	34	M34G	0.6402366074	1
## 367	34	M34Q	0.9456588852	1
## 368	34	M34Y	0.8952467009	1
## 369	34	M34S	0.8220752140	1
## 370	34	M34V	0.6543453822	1
## 371	34	M34W	0.5759299985	0
## 372	34	M34A	0.7563449481	1
## 373	34	M34T	1.1658001233	1
## 374	34	M34R	0.6639621429	1
## 375	34	M34D	0.4826683868	0
## 376	35	R35G	1.1722625007	1
## 377	36	R36C	0.7925392936	1
## 378	36	R36A	0.9240664133	1
## 379	36	R36S	0.6429017966	1
## 380	36	R36T	0.4723056809	0
## 381	36	R36P	-0.1182932658	0
## 382	36	R36Q	0.9639217040	1
## 383	36	R36G	0.6507615025	1
## 384	36	R36H	0.7605625642	1
## 385	36	R36E	0.4297964625	0
## 386	36	R36F	0.8944696260	1

## 387	36	R36L	0.6807406446	1
## 388	36	R36M	0.5878060688	0
## 389	36	R36N	0.9338524560	1
## 390	36	R36I	0.7388076851	1
## 391	36	R36K	0.7717513918	1
## 392	36	R36V	0.8180937852	1
## 393	36	R36Y	0.7595547029	1
## 394	37	M37Y	0.8780558553	1
## 395	37	M37D	-0.2746587623	0
## 396	37	M37V	0.7199930861	1
## 397	37	M37W	0.5499007721	0
## 398	37	M37E	0.0246480088	0
## 399	37	M37F	0.6978764936	1
## 400	37	M37A	0.6674849879	1
## 401	37	M37C	0.4219754253	0
## 402	37	M37S	-0.0023606078	0
## 403	37	M37T	0.2087763419	0
## 404	37	M37I	1.0146204455	1
## 405	37	M37R	-0.0768044588	0
## 406	37	M37Q	0.2152961974	0
## 407	37	M37H	-0.3255836015	0
## 408	37	M37L	0.8355446447	1
## 409	37	M37G	0.1847536112	0
## 410	37	M37N	-0.5324461818	0
## 411	37	M37P	-0.0656289266	0
## 412	38	Q38C	0.8741532093	1
## 413	38	Q38G	0.7754357064	1
## 414	38	Q38D	0.5440520389	0
## 415	38	Q38E	0.4118405870	0
## 416	38	Q38A	0.7847327465	1
## 417	38	Q38S	0.3626857985	0
## 418	38	Q38T	0.1116319640	0
## 419	38	Q38F	0.6107066086	1
## 420	38	Q38W	1.0220742155	1
## 421	38	Q38Y	0.6600626360	1
## 422	38	Q38H	1.0422360604	1
## 423	38	Q38V	0.7925041025	1
## 424	38	Q38P	0.1067863237	0
## 425	38	Q38R	0.9798222112	1
## 426	38	Q38L	0.7555725892	1
## 427	38	Q38M	0.9218353738	1
## 428	38	Q38I	0.9627428608	1
## 429	38	Q38K	0.9898266147	1
## 430	38	Q38N	0.6868160801	1
## 431	39	K39V	1.0492264120	1
## 432	39	K39W	0.7928790519	1
## 433	39	K39F	0.6391805089	1
## 434	39	K39T	0.9585416528	1
## 435	39	K39H	0.9813163558	1
## 436	39	K39E	1.1029375058	1
## 437	39	K39G	0.6744491869	1
## 438	39	K39D	1.0728311729	1
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## 440	39	K39N	1.0674308041	1

## 441	39	K39Y	1.1926906377	1
## 442	39	K39C	0.8358382355	1
## 443	39	K39I	0.6152220839	1
## 444	39	K39L	0.8426672765	1
## 445	39	K39S	0.8905194326	1
## 446	39	K39P	-0.1402407862	0
## 447	39	K39R	0.8305114741	1
## 448	39	K39A	0.9403023027	1
## 449	39	K39Q	0.9255872966	1
## 450	40	E40K	0.2943710917	0
## 451	40	E40H	0.2743403667	0
## 452	40	E40G	0.4229737312	0
## 453	40	E40F	0.0780488492	0
## 454	40	E40M	0.8020455793	1
## 455	40	E40I	0.2607674798	0
## 456	40	E40N	0.6592129012	1
## 457	40	E40L	-0.1269854613	0
## 458	40	E40P	-0.1087347295	0
## 459	40	E40A	0.7878951079	1
## 460	40	E40D	1.0618119533	1
## 461	40	E40R	-0.0669344987	0
## 462	40	E40C	0.2577890259	0
## 463	40	E40S	0.7046974554	1
## 464	40	E40Y	0.0550933009	0
## 465	40	E40W	0.3055253526	0
## 466	40	E40T	0.6587295024	1
## 467	40	E40V	0.7757991854	1
## 468	41	M41D	0.3658744705	0
## 469	41	M41C	0.7077255867	1
## 470	41	M41E	0.1143714364	0
## 471	41	M41G	0.1989501402	0
## 472	41	M41T	0.6760629384	1
## 473	41	M41F	1.1152391348	1
## 474	41	M41A	0.0897107457	0
## 475	41	M41R	0.0592483573	0
## 476	41	M41S	0.2333800560	0
## 477	41	M41V	0.6705763999	1
## 478	41	M41W	-0.0063376827	0
## 479	41	M41Q	0.5340242536	0
## 480	41	M41Y	0.8956867550	1
## 481	41	M41H	-0.1201131183	0
## 482	41	M41L	0.8049339976	1
## 483	41	M41P	-0.1040669335	0
## 484	42	D42V	0.9910339196	1
## 485	42	D42S	0.8223783711	1
## 486	42	D42P	0.0395961599	0
## 487	42	D42M	0.7260641664	1
## 488	42	D42Q	1.2318019946	1
## 489	42	D42W	1.1888221837	1
## 490	42	D42Y	0.8252784838	1
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## 492	42	D42L	1.0882070314	1
## 493	42	D42R	0.8859027804	1
## 494	42	D42N	1.0850246715	1

## 495	42	D42C	1.0233267403	1
## 496	42	D42I	0.6118055352	1
## 497	42	D42A	0.8751865003	1
## 498	42	D42G	0.9249727686	1
## 499	42	D42F	0.9485813770	1
## 500	42	D42T	0.7726936056	1
## 501	42	D42E	0.8495331276	1
## 502	43	R43A	0.7722230643	1
## 503	43	R43P	0.1295757715	0
## 504	43	R43L	1.1483871327	1
## 505	43	R43M	0.9433628623	1
## 506	43	R43N	0.9071535641	1
## 507	43	R43E	0.9407648349	1
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## 511	43	R43I	0.7052281567	1
## 512	43	R43K	1.2253453727	1
## 513	43	R43F	0.9446101800	1
## 514	43	R43G	0.5690323669	0
## 515	43	R43T	0.4217523621	0
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## 520	44	G44K	0.0851786544	0
## 521	44	G44I	0.3857692878	0
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## 525	44	G44M	0.0602837640	0
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## 529	44	G44E	0.1845071854	0
## 530	44	G44L	0.2034844821	0
## 531	44	G44T	-0.1293125056	0
## 532	44	G44S	0.4743010400	0
## 533	44	G44P	-0.2066524934	0
## 534	44	G44R	0.0157614331	0
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## 537	45	L45S	0.2241760871	0
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## 540	45	L45R	0.4169266332	0
## 541	45	L45D	-0.5469391234	0
## 542	45	L45W	0.3106111145	0
## 543	45	L45C	0.6698851057	1
## 544	45	L45I	0.5165937338	0
## 545	45	L45V	0.6644212026	1
## 546	45	L45Q	0.2274280553	0
## 547	45	L45H	0.3632631395	0
## 548	45	L45G	-0.0961551844	0

## 549	45	L45E	0.2828847126	0
## 550	45	L45P	-0.0406426793	0
## 551	45	L45K	0.1924193907	0
## 552	45	L45Y	-0.0967679992	0
## 553	45	L45N	0.2534222346	0
## 554	46	R46E	0.7415907803	1
## 555	46	R46A	1.1181687190	1
## 556	46	R46C	0.8235967067	1
## 557	46	R46D	0.7842073011	1
## 558	46	R46T	0.8177558795	1
## 559	46	R46P	-0.0275672305	0
## 560	46	R46Q	0.6707422356	1
## 561	46	R46S	0.9629913622	1
## 562	46	R46H	0.7293784406	1
## 563	46	R46V	0.5738506596	0
## 564	46	R46F	0.6017257031	1
## 565	46	R46G	1.0227525938	1
## 566	46	R46M	1.1177484226	1
## 567	46	R46N	0.7249352301	1
## 568	46	R46I	0.5566140512	0
## 569	46	R46K	0.7879795669	1
## 570	46	R46W	-0.0579545052	0
## 571	46	R46Y	0.4958412256	0
## 572	46	R46L	0.7980444932	1
## 573	47	L47H	0.5590572150	0
## 574	47	L47G	1.1724518784	1
## 575	47	L47Y	1.1362960272	1
## 576	47	L47W	0.4995364275	0
## 577	47	L47K	1.0624841869	1
## 578	47	L47I	0.8497506633	1
## 579	47	L47D	1.2961400000	1
## 580	47	L47E	1.0339028207	1
## 581	47	L47F	0.9761658181	1
## 582	47	L47V	0.9917913188	1
## 583	47	L47T	0.8933713582	1
## 584	47	L47Q	1.1450013386	1
## 585	47	L47P	0.4568038530	0
## 586	47	L47R	0.8967179560	1
## 587	47	L47M	1.0480114807	1
## 588	47	L47A	0.4968690093	0
## 589	47	L47S	0.8806094137	1
## 590	47	L47N	0.8993532260	1
## 591	47	L47C	1.0021984194	1
## 592	48	E48N	0.7887949527	1
## 593	48	E48S	1.0222778823	1
## 594	48	E48D	0.9453581906	1
## 595	48	E48L	0.4270467516	0
## 596	48	E48P	0.7326617216	1
## 597	48	E48G	0.7247025255	1
## 598	48	E48H	0.6110643438	1
## 599	48	E48I	1.0640112481	1
## 600	48	E48R	0.5460827882	0
## 601	48	E48T	0.6239748397	1
## 602	48	E48V	0.8198187593	1

## 603	48	E48A	0.8406672896	1
## 604	49	T49A	0.5815283123	0
## 605	49	T49C	0.6346559224	1
## 606	49	T49D	0.6899020645	1
## 607	49	T49E	0.5384627552	0
## 608	49	T49F	0.8444177702	1
## 609	49	T49G	0.5377272259	0
## 610	49	T49H	0.8642818931	1
## 611	49	T49I	0.5256001642	0
## 612	49	T49K	0.7083270420	1
## 613	49	T49L	0.8373154797	1
## 614	49	T49M	0.1797888521	0
## 615	49	T49N	0.6444371010	1
## 616	49	T49P	0.5673930731	0
## 617	49	T49Q	0.6313896898	1
## 618	49	T49R	0.3671152691	0
## 619	49	T49S	0.6340529865	1
## 620	49	T49V	0.5257954864	0
## 621	49	T49W	0.2784872786	0
## 622	50	H50D	0.5567433231	0
## 623	50	H50A	0.5024099618	0
## 624	50	H50E	0.9319691888	1
## 625	50	H50C	0.8154190348	1
## 626	50	H50V	0.8650749610	1
## 627	50	H50R	1.2125098261	1
## 628	50	H50W	0.8313332456	1
## 629	50	H50F	0.4173207395	0
## 630	50	H50I	0.9594679878	1
## 631	50	H50T	0.7867997125	1
## 632	50	H50Q	1.0420767965	1
## 633	50	H50G	0.4196061241	0
## 634	50	H50Y	0.9970074745	1
## 635	50	H50M	0.9287045754	1
## 636	50	H50K	0.7149614974	1
## 637	50	H50S	0.2385843648	0
## 638	50	H50P	0.3922679252	0
## 639	50	H50L	0.5753805032	0
## 640	51	E51M	0.8888564436	1
## 641	51	E51K	0.8694178783	1
## 642	51	E51R	1.1311300010	1
## 643	51	E51H	1.3644154731	1
## 644	51	E51L	0.8163068004	1
## 645	51	E51W	0.8567927439	1
## 646	51	E51I	0.5322687094	0
## 647	51	E51S	0.6565976491	1
## 648	51	E51T	1.0378290900	1
## 649	51	E51V	0.5059500591	0
## 650	51	E51A	1.0166323705	1
## 651	51	E51G	0.9452568784	1
## 652	51	E51N	0.2440735706	0
## 653	51	E51P	0.8723305268	1
## 654	51	E51Q	0.7973384701	1
## 655	51	E51F	0.7614615395	1
## 656	51	E51Y	0.3152591799	0

## 657	51	E51C	1.2745745772	1
## 658	52	E52R	0.8341581192	1
## 659	52	E52K	1.2486794850	1
## 660	52	E52Y	0.8670043995	1
## 661	52	E52L	0.9267082800	1
## 662	52	E52Q	1.0778507789	1
## 663	52	E52T	1.1104846752	1
## 664	52	E52W	0.8546117739	1
## 665	52	E52M	0.8691267676	1
## 666	52	E52I	0.7448597930	1
## 667	52	E52S	0.9827579416	1
## 668	52	E52P	0.2433509951	0
## 669	52	E52C	1.0968205982	1
## 670	52	E52H	0.7347472739	1
## 671	52	E52G	1.1915405816	1
## 672	52	E52A	0.6873921123	1
## 673	52	E52D	0.4784342137	0
## 674	52	E52F	1.1291437057	1
## 675	52	E52V	0.7633434426	1
## 676	53	A53H	0.3442254924	0
## 677	53	A53M	0.6115310296	1
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## 679	53	A53T	0.8215966442	1
## 680	53	A53W	-0.1340005473	0
## 681	53	A53V	0.5661446703	0
## 682	53	A53Q	0.0444324520	0
## 683	53	A53G	0.5166021671	0
## 684	53	A53N	0.3190719976	0
## 685	53	A53P	0.1237514797	0
## 686	53	A53K	0.4383953414	0
## 687	53	A53I	0.1298313345	0
## 688	53	A53S	0.4391162058	0
## 689	53	A53C	0.7908653318	1
## 690	53	A53E	0.0278523340	0
## 691	53	A53F	0.4289089542	0
## 692	53	A53Y	0.1810865140	0
## 693	53	A53R	0.3455978376	0
## 694	54	S54A	0.9587623173	1
## 695	54	S54C	1.0114727287	1
## 696	54	S54D	1.0691169346	1
## 697	54	S54E	0.8522858773	1
## 698	54	S54F	0.3522610439	0
## 699	54	S54G	0.8917213875	1
## 700	54	S54H	0.9791275703	1
## 701	54	S54I	0.6184774556	1
## 702	54	S54K	1.0610609001	1
## 703	54	S54L	0.7331346230	1
## 704	54	S54M	0.9263861832	1
## 705	54	S54P	0.8103620267	1
## 706	54	S54Q	0.7728859221	1
## 707	54	S54R	0.6446118603	1
## 708	54	S54T	0.9511729117	1
## 709	54	S54V	1.0714782458	1
## 710	54	S54W	0.6254913562	1

## 711	54	S54Y	0.2008972846	0
## 712	55	V55A	0.2662771863	0
## 713	55	V55C	0.9800482708	1
## 714	55	V55E	0.0221266162	0
## 715	55	V55G	0.1078632232	0
## 716	55	V55H	-0.1761208430	0
## 717	55	V55K	-0.1240897221	0
## 718	55	V55L	0.8632521524	1
## 719	55	V55M	1.1000127587	1
## 720	55	V55N	0.0853024622	0
## 721	55	V55P	0.1876402109	0
## 722	55	V55Q	-0.2018352898	0
## 723	55	V55R	0.1429068133	0
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## 725	55	V55T	0.6955318793	1
## 726	55	V55W	0.1911190531	0
## 727	55	V55Y	0.1199358473	0
## 728	56	K56R	0.9010942976	1
## 729	56	K56S	0.8340106739	1
## 730	56	K56Q	0.9772489899	1
## 731	56	K56G	0.9309663285	1
## 732	56	K56C	0.4010632425	0
## 733	56	K56E	0.1587772866	0
## 734	56	K56F	0.4291808468	0
## 735	56	K56A	0.7051812497	1
## 736	56	K56P	0.7744741299	1
## 737	56	K56H	0.4538430223	0
## 738	56	K56D	0.0617466832	0
## 739	56	K56T	0.4725068314	0
## 740	56	K56V	0.7775331909	1
## 741	56	K56W	0.2980216976	0
## 742	56	K56I	0.9307934725	1
## 743	56	K56L	0.8489608756	1
## 744	56	K56Y	0.1876243159	0
## 745	57	M57H	0.3519751452	0
## 746	57	M57I	0.5627807025	0
## 747	57	M57G	-0.0695290132	0
## 748	57	M57W	0.1320906387	0
## 749	57	M57F	0.2680351717	0
## 750	57	M57N	-0.2031207860	0
## 751	57	M57P	0.2541704587	0
## 752	57	M57L	0.5644112274	0
## 753	57	M57E	-0.1176810845	0
## 754	57	M57A	-0.3552365230	0
## 755	57	M57C	0.7189724636	1
## 756	57	M57Y	0.4058861137	0
## 757	57	M57D	-0.2721819026	0
## 758	57	M57T	-0.0643573268	0
## 759	57	M57V	0.3799616525	0
## 760	57	M57R	0.1150488318	0
## 761	57	M57S	0.1832874765	0
## 762	57	M57Q	0.5459972455	0
## 763	58	L58A	0.5416838699	0
## 764	58	L58C	0.8513011335	1

## 765	58	L58E	0.9174250856	1
## 766	58	L58P	-0.4156473970	0
## 767	58	L58D	1.0368899053	1
## 768	58	L58K	0.9358074410	1
## 769	58	L58N	0.9650778237	1
## 770	58	L58Q	1.1144490943	1
## 771	58	L58R	0.7932724692	1
## 772	58	L58I	0.9135756198	1
## 773	58	L58S	0.6956928582	1
## 774	58	L58T	0.5189524284	0
## 775	58	L58V	1.0058087170	1
## 776	58	L58F	0.9162400565	1
## 777	58	L58G	0.7608462275	1
## 778	58	L58H	0.7561041341	1
## 779	58	L58Y	1.3379441436	1
## 780	58	L58W	0.9964041866	1
## 781	59	P59K	0.3906353317	0
## 782	59	P59M	0.4812564965	0
## 783	59	P59N	-0.0997246560	0
## 784	59	P59Q	0.4280768945	0
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## 786	59	P59F	0.3994577601	0
## 787	59	P59G	0.0363243210	0
## 788	59	P59H	0.6769442272	1
## 789	59	P59R	0.2525980638	0
## 790	59	P59W	0.6425729963	1
## 791	59	P59S	0.7208864758	1
## 792	59	P59T	0.7152501817	1
## 793	59	P59I	-0.7723840320	0
## 794	59	P59V	0.4742007751	0
## 795	59	P59D	0.7509714003	1
## 796	59	P59E	1.1164862782	1
## 797	59	P59A	0.8201651627	1
## 798	59	P59C	-0.0148188964	0
## 799	60	T60A	0.4231065748	0
## 800	60	T60C	1.0809924737	1
## 801	60	T60D	0.2763463415	0
## 802	60	T60E	0.4389407644	0
## 803	60	T60F	0.5667022002	0
## 804	60	T60G	0.4753787504	0
## 805	60	T60H	0.4300618813	0
## 806	60	T60K	-0.2371309924	0
## 807	60	T60L	0.5849554436	0
## 808	60	T60M	0.7462323723	1
## 809	60	T60P	0.4716758500	0
## 810	60	T60Q	0.1166636024	0
## 811	60	T60R	0.1682600708	0
## 812	60	T60S	0.7266185414	1
## 813	60	T60V	0.7059566764	1
## 814	60	T60W	0.3559158171	0
## 815	60	T60Y	0.3872929915	0
## 816	61	Y61A	0.6678289788	1
## 817	61	Y61C	0.9552152695	1
## 818	61	Y61D	0.9667616404	1

## 819	61	Y61E	0.7888929584	1
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## 821	61	Y61G	0.9036949770	1
## 822	61	Y61H	0.7495456219	1
## 823	61	Y61I	0.9895109539	1
## 824	61	Y61K	0.5517701736	0
## 825	61	Y61L	0.9394988231	1
## 826	61	Y61M	0.4980604408	0
## 827	61	Y61N	0.5499533570	0
## 828	61	Y61P	0.7450214203	1
## 829	61	Y61Q	0.8401551901	1
## 830	61	Y61R	0.6130173969	1
## 831	61	Y61S	0.9797313487	1
## 832	61	Y61T	0.3725059085	0
## 833	61	Y61V	0.6274198357	1
## 834	61	Y61W	0.9425618721	1
## 835	62	V62A	0.5808842809	0
## 836	62	V62C	1.0495307328	1
## 837	62	V62E	0.4732422705	0
## 838	62	V62F	0.8055024229	1
## 839	62	V62G	0.4182525255	0
## 840	62	V62H	0.9702992282	1
## 841	62	V62I	0.7670534614	1
## 842	62	V62K	-0.1031413560	0
## 843	62	V62L	0.6762854065	1
## 844	62	V62M	0.4950709774	0
## 845	62	V62N	0.3034723479	0
## 846	62	V62P	0.2915923055	0
## 847	62	V62Q	0.0810925622	0
## 848	62	V62R	0.3159766771	0
## 849	62	V62S	0.2552564290	0
## 850	62	V62T	0.2013757291	0
## 851	62	V62W	0.7627135962	1
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## 853	63	R63A	1.0443373440	1
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## 855	63	R63E	1.0583358480	1
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## 860	63	R63P	-0.0477254502	0
## 861	63	R63Q	0.3359918980	0
## 862	63	R63S	1.0725734656	1
## 863	63	R63T	0.8664978282	1
## 864	63	R63V	0.8561202243	1
## 865	63	R63W	0.6458660852	1
## 866	63	R63Y	0.9592266387	1
## 867	63	R63H	0.8058509836	1
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## 872	64	S64A	1.1280800092	1

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## 890	65	T65A	0.7336777260	1
## 891	65	T65C	1.0023900667	1
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## 895	65	T65H	0.7021886464	1
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## 902	65	T65Q	1.0189300519	1
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## 908	66	P66I	1.2561126286	1
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## 912	66	P66G	0.8411228902	1
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## 914	66	P66V	0.9596330872	1
## 915	66	P66E	0.6793469426	1
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## 917	66	P66T	0.7853906688	1
## 918	66	P66L	0.8317217365	1
## 919	66	P66W	0.5363576808	0
## 920	66	P66Y	0.9348767191	1
## 921	66	P66C	0.8551503525	1
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## 923	66	P66R	0.9650576363	1
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## 932	67	E67S	0.7837938756	1
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## 936	67	E67Y	0.8555840879	1
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## 950	68	G68H	0.8994842552	1
## 951	68	G68R	0.8214996726	1
## 952	68	G68W	0.7779561984	1
## 953	68	G68K	0.8481453673	1
## 954	68	G68T	1.1343922451	1
## 955	68	G68V	0.8917283750	1
## 956	68	G68Y	0.8969617605	1
## 957	68	G68M	0.6221990654	1
## 958	68	G68L	0.9847167891	1
## 959	68	G68F	0.9950370105	1
## 960	68	G68C	0.7643266528	1
## 961	68	G68A	0.8279586588	1
## 962	68	G68E	1.1212323060	1
## 963	69	S69A	0.8895843617	1
## 964	69	S69C	0.7168822468	1
## 965	69	S69D	1.0931248177	1
## 966	69	S69E	0.4540495365	0
## 967	69	S69F	0.7805895681	1
## 968	69	S69G	0.9071614334	1
## 969	69	S69H	0.9907679312	1
## 970	69	S69I	0.9854631517	1
## 971	69	S69K	0.7505748425	1
## 972	69	S69L	0.9575714990	1
## 973	69	S69M	1.1440406201	1
## 974	69	S69N	1.0467245721	1
## 975	69	S69P	1.0273842686	1
## 976	69	S69Q	0.4613181003	0
## 977	69	S69R	0.7104315187	1
## 978	69	S69T	0.8800126685	1
## 979	69	S69V	0.9452084483	1
## 980	69	S69W	1.0070978807	1

## 981	69	S69Y	1.0434305342	1
## 982	70	E70W	0.6583923158	1
## 983	70	E70F	0.7260103576	1
## 984	70	E70S	0.9954407707	1
## 985	70	E70G	0.9518813505	1
## 986	70	E70T	1.3492696347	1
## 987	70	E70V	0.7271083096	1
## 988	70	E70Y	0.9934984295	1
## 989	70	E70C	0.5864940161	0
## 990	70	E70H	0.8725452702	1
## 991	70	E70A	0.9333386166	1
## 992	70	E70R	1.0810865361	1
## 993	70	E70Q	0.7582863651	1
## 994	70	E70M	0.5726750970	0
## 995	70	E70L	0.3651281347	0
## 996	70	E70I	0.6703850949	1
## 997	70	E70P	0.7654425843	1
## 998	70	E70N	1.2953786260	1
## 999	70	E70K	1.1490992563	1
## 1000	71	V71A	0.9946321429	1
## 1001	71	V71C	1.0908809209	1
## 1002	71	V71D	0.1513371802	0
## 1003	71	V71E	0.9569695372	1
## 1004	71	V71F	0.6585431219	1
## 1005	71	V71G	0.8520987160	1
## 1006	71	V71H	0.3999389002	0
## 1007	71	V71K	0.5946488716	0
## 1008	71	V71L	0.7460460498	1
## 1009	71	V71M	1.1531123846	1
## 1010	71	V71N	1.2015118227	1
## 1011	71	V71P	0.4950509555	0
## 1012	71	V71Q	1.5467522713	1
## 1013	71	V71R	0.8738778102	1
## 1014	71	V71S	0.7750687927	1
## 1015	71	V71T	0.8545365368	1
## 1016	71	V71W	0.3645433633	0
## 1017	71	V71Y	0.4362732899	0
## 1018	72	G72M	-0.0613894414	0
## 1019	72	G72T	0.5319238755	0
## 1020	72	G72V	0.4459197135	0
## 1021	72	G72Q	0.2615713784	0
## 1022	72	G72L	0.1387763503	0
## 1023	72	G72S	0.3045026263	0
## 1024	72	G72P	0.3693335121	0
## 1025	72	G72A	0.3137319071	0
## 1026	72	G72W	0.4281451373	0
## 1027	72	G72N	-0.1408446857	0
## 1028	72	G72Y	0.2018533221	0
## 1029	72	G72E	0.6684546283	1
## 1030	72	G72I	0.3335329424	0
## 1031	72	G72R	0.1679191210	0
## 1032	72	G72F	0.4058931416	0
## 1033	72	G72K	0.6263115084	1
## 1034	72	G72D	0.9836888221	1

## 1035	72	G72H	0.7693131237	1
## 1036	73	D73V	0.1705764779	0
## 1037	73	D73S	0.4381527984	0
## 1038	73	D73T	0.7042829920	1
## 1039	73	D73C	0.0727642328	0
## 1040	73	D73A	0.4400179647	0
## 1041	73	D73F	0.2852362077	0
## 1042	73	D73Y	0.2524797625	0
## 1043	73	D73G	0.4500839087	0
## 1044	73	D73H	0.4626759048	0
## 1045	73	D73E	0.6394229582	1
## 1046	73	D73K	0.2339921646	0
## 1047	73	D73R	0.4219761359	0
## 1048	73	D73I	0.1521562238	0
## 1049	73	D73W	0.1777099536	0
## 1050	73	D73M	0.3389948160	0
## 1051	73	D73Q	0.4611311187	0
## 1052	73	D73N	0.6926775711	1
## 1053	73	D73L	0.6799171491	1
## 1054	73	D73P	0.1415322607	0
## 1055	74	F74D	0.1950832618	0
## 1056	74	F74Y	1.1378530694	1
## 1057	74	F74H	0.9873832712	1
## 1058	74	F74V	0.9606365722	1
## 1059	74	F74G	0.6389285727	1
## 1060	74	F74S	0.7009180487	1
## 1061	74	F74A	0.9265243000	1
## 1062	74	F74E	0.1647780697	0
## 1063	74	F74T	0.9813446415	1
## 1064	74	F74Q	0.5178104606	0
## 1065	74	F74R	0.1868474393	0
## 1066	74	F74N	0.4377993403	0
## 1067	74	F74C	0.6999798587	1
## 1068	74	F74P	0.0916817430	0
## 1069	74	F74M	1.0738431100	1
## 1070	74	F74K	0.6401741317	1
## 1071	74	F74W	0.4738196155	0
## 1072	74	F74I	0.2342371896	0
## 1073	74	F74L	0.8465131622	1
## 1074	75	L75H	0.4312322534	0
## 1075	75	L75I	0.4672330161	0
## 1076	75	L75E	0.1248269034	0
## 1077	75	L75F	0.4739649363	0
## 1078	75	L75K	0.2696383633	0
## 1079	75	L75A	0.5489229939	0
## 1080	75	L75M	0.8367924030	1
## 1081	75	L75G	0.2452686854	0
## 1082	75	L75D	0.6361673579	1
## 1083	75	L75P	0.2644088916	0
## 1084	75	L75T	0.3700044123	0
## 1085	75	L75V	0.7955874201	1
## 1086	75	L75N	0.0619059478	0
## 1087	75	L75Y	0.3169262334	0
## 1088	75	L75C	0.6225709365	1

## 1089	75	L75Q	0.2198395862	0
## 1090	75	L75R	0.3924216556	0
## 1091	75	L75W	0.4708491576	0
## 1092	75	L75S	0.5081564469	0
## 1093	76	S76A	0.8363130149	1
## 1094	76	S76C	0.6372722248	1
## 1095	76	S76D	0.6167483980	1
## 1096	76	S76E	0.8760118443	1
## 1097	76	S76F	0.7572220024	1
## 1098	76	S76G	0.9314964433	1
## 1099	76	S76H	0.6870409046	1
## 1100	76	S76K	0.7274809920	1
## 1101	76	S76L	0.5442462691	0
## 1102	76	S76M	0.6883606236	1
## 1103	76	S76N	0.9060773656	1
## 1104	76	S76P	0.6203009159	1
## 1105	76	S76Q	0.7492419096	1
## 1106	76	S76R	0.6438216393	1
## 1107	76	S76T	0.6554412594	1
## 1108	76	S76V	0.9742337554	1
## 1109	76	S76W	0.6282090006	1
## 1110	76	S76Y	0.8230732415	1
## 1111	77	L77D	0.6708418836	1
## 1112	77	L77F	0.7600704684	1
## 1113	77	L77G	0.9029152119	1
## 1114	77	L77C	1.1571255049	1
## 1115	77	L77H	0.7087075592	1
## 1116	77	L77E	0.4029486594	0
## 1117	77	L77S	0.6059617744	1
## 1118	77	L77T	0.7323032039	1
## 1119	77	L77P	0.4656532000	0
## 1120	77	L77Q	0.1780107392	0
## 1121	77	L77R	0.1923313180	0
## 1122	77	L77A	1.1449668091	1
## 1123	77	L77N	0.5275849880	0
## 1124	77	L77V	0.9557890865	1
## 1125	77	L77W	0.8847416267	1
## 1126	77	L77Y	0.5732137147	0
## 1127	77	L77M	0.8159832956	1
## 1128	77	L77I	0.8278043977	1
## 1129	77	L77K	0.1941536649	0
## 1130	86	V86A	0.7991373095	1
## 1131	86	V86C	0.8469941674	1
## 1132	86	V86D	0.4719385624	0
## 1133	86	V86E	0.6441888229	1
## 1134	86	V86F	0.7064873518	1
## 1135	86	V86G	0.6956584451	1
## 1136	86	V86H	-0.0885292051	0
## 1137	86	V86I	0.5783720678	0
## 1138	86	V86K	0.6622988428	1
## 1139	86	V86L	0.8698337630	1
## 1140	86	V86M	0.7193894170	1
## 1141	86	V86N	0.8015207469	1
## 1142	86	V86P	0.5446526200	0

## 1143	86	V86Q	0.6827869151	1
## 1144	86	V86R	0.3292370525	0
## 1145	86	V86S	0.8386532936	1
## 1146	86	V86T	0.7810445508	1
## 1147	86	V86W	0.4782607082	0
## 1148	86	V86Y	0.7395111207	1
## 1149	87	M87Y	1.0677307075	1
## 1150	87	M87V	0.9784725854	1
## 1151	87	M87W	1.2605604490	1
## 1152	87	M87A	0.7405345759	1
## 1153	87	M87C	0.9085650607	1
## 1154	87	M87D	0.5842381043	0
## 1155	87	M87E	0.6920162401	1
## 1156	87	M87F	0.7708236763	1
## 1157	87	M87R	0.5775296761	0
## 1158	87	M87S	0.6500402626	1
## 1159	87	M87T	0.5440613302	0
## 1160	87	M87I	0.6639547030	1
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## 1162	87	M87G	0.7144744540	1
## 1163	87	M87H	0.6694415881	1
## 1164	87	M87P	0.6391049463	1
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## 1167	88	L88K	0.4903413088	0
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## 1171	88	L88F	0.5887961410	0
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## 1176	88	L88Y	0.8947839894	1
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## 1183	88	L88R	0.4999422761	0
## 1184	88	L88N	1.0680153670	1
## 1185	89	V89A	0.8237261085	1
## 1186	89	V89C	0.6337087060	1
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## 1188	89	V89F	0.7728259172	1
## 1189	89	V89G	0.4308819112	0
## 1190	89	V89H	0.6894317880	1
## 1191	89	V89I	1.1153056161	1
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## 1193	89	V89L	0.8021778938	1
## 1194	89	V89M	0.6689830718	1
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## 1196	89	V89P	0.2170972054	0

## 1197	89	V89Q	0.4150897679	0
## 1198	89	V89R	0.2242146320	0
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## 1202	89	V89Y	0.5301401264	0
## 1203	90	K90E	0.7396880059	1
## 1204	90	K90C	0.8632077593	1
## 1205	90	K90H	0.6211765565	1
## 1206	90	K90Y	0.5782307106	0
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## 1210	90	K90D	0.7008221876	1
## 1211	90	K90W	0.8100915579	1
## 1212	90	K90T	0.9151720559	1
## 1213	90	K90R	0.8485805621	1
## 1214	90	K90V	0.8705038818	1
## 1215	90	K90L	0.8808122495	1
## 1216	90	K90M	0.6745280662	1
## 1217	90	K90Q	0.9632083718	1
## 1218	90	K90I	0.6744105665	1
## 1219	90	K90A	0.8576686900	1
## 1220	90	K90S	0.8203237040	1
## 1221	90	K90P	0.4472973360	0
## 1222	91	V91A	0.9193862913	1
## 1223	91	V91C	1.1909359679	1
## 1224	91	V91D	0.5427079514	0
## 1225	91	V91E	0.7430009482	1
## 1226	91	V91F	0.9628332318	1
## 1227	91	V91G	0.7801885790	1
## 1228	91	V91H	0.7918378440	1
## 1229	91	V91I	0.9810985284	1
## 1230	91	V91K	0.5181868366	0
## 1231	91	V91L	0.9954707664	1
## 1232	91	V91M	0.9765184176	1
## 1233	91	V91N	0.6976656800	1
## 1234	91	V91P	0.4555370710	0
## 1235	91	V91Q	0.7458980929	1
## 1236	91	V91R	0.5205317649	0
## 1237	91	V91S	0.9988449233	1
## 1238	91	V91T	0.9692467347	1
## 1239	91	V91W	0.5174300106	0
## 1240	91	V91Y	0.6261075560	1
## 1241	92	G92T	1.0233000433	1
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## 1243	92	G92E	0.8049740598	1
## 1244	92	G92R	0.8148256979	1
## 1245	92	G92C	0.8910876625	1
## 1246	92	G92I	0.8866510831	1
## 1247	92	G92L	0.8887089693	1
## 1248	92	G92Q	0.8274970210	1
## 1249	92	G92H	0.6845288665	1
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## 1257	92	G92M	0.7802092568	1
## 1258	92	G92A	0.8014422358	1
## 1259	93	E93W	0.8289303127	1
## 1260	93	E93D	0.9908511611	1
## 1261	93	E93V	1.0444662562	1
## 1262	93	E93L	1.0597024113	1
## 1263	93	E93H	1.1657795433	1
## 1264	93	E93Y	1.1283502170	1
## 1265	93	E93K	1.2122565130	1
## 1266	93	E93G	1.0030371793	1
## 1267	93	E93S	0.9626131656	1
## 1268	93	E93F	1.0581709970	1
## 1269	93	E93T	0.9858627142	1
## 1270	93	E93A	0.8084141650	1
## 1271	93	E93R	0.9089525922	1
## 1272	93	E93M	0.9273703391	1
## 1273	93	E93I	0.8656513304	1
## 1274	93	E93C	0.9672190035	1
## 1275	93	E93N	1.0873917325	1
## 1276	93	E93Q	0.7732514908	1
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## 1278	94	G94C	0.8208735409	1
## 1279	94	G94Y	0.8949068813	1
## 1280	94	G94W	0.9204912350	1
## 1281	94	G94F	0.9762868136	1
## 1282	94	G94I	0.7472227357	1
## 1283	94	G94K	0.4706614338	0
## 1284	94	G94V	0.9029506101	1
## 1285	94	G94D	0.7518761879	1
## 1286	94	G94E	0.8274697256	1
## 1287	94	G94M	0.6618496593	1
## 1288	94	G94T	0.7270851102	1
## 1289	94	G94A	1.0173603015	1
## 1290	94	G94L	0.8906239052	1
## 1291	94	G94P	0.6612417665	1
## 1292	94	G94R	0.9292160289	1
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## 1296	95	E95K	0.7413666795	1
## 1297	95	E95Y	1.0857570227	1
## 1298	95	E95D	1.0045258762	1
## 1299	95	E95A	0.8338216282	1
## 1300	95	E95F	0.9190441459	1
## 1301	95	E95I	1.1195500054	1
## 1302	95	E95H	0.6918534442	1
## 1303	95	E95L	0.9941611643	1
## 1304	95	E95W	0.7834448616	1

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## 1306	95	E95C	1.2089408653	1
## 1307	95	E95M	1.0222151021	1
## 1308	95	E95N	0.5592223746	0
## 1309	95	E95G	0.9964826812	1
## 1310	95	E95R	0.8633209913	1
## 1311	95	E95S	1.0312727096	1
## 1312	95	E95Q	0.7095903523	1
## 1313	95	E95V	1.1041758907	1
## 1314	95	E95P	0.9985882306	1
## 1315	96	E96Y	1.0538533695	1
## 1316	96	E96C	1.0646666258	1
## 1317	96	E96P	0.7201492821	1
## 1318	96	E96I	0.6088482218	1
## 1319	96	E96H	0.8992028603	1
## 1320	96	E96L	0.9797126292	1
## 1321	96	E96D	1.0144317214	1
## 1322	96	E96A	0.8630367013	1
## 1323	96	E96W	0.8977161327	1
## 1324	96	E96F	1.1609255405	1
## 1325	96	E96G	1.0149018748	1
## 1326	96	E96K	1.1327858850	1
## 1327	96	E96N	0.9364626807	1
## 1328	96	E96T	1.0295655448	1
## 1329	96	E96S	1.0531642458	1
## 1330	96	E96Q	0.9498023714	1
## 1331	96	E96V	0.9526150621	1
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## 1333	96	E96M	0.9274215316	1
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## 1335	97	G97D	0.7469121331	1
## 1336	97	G97L	0.9032379439	1
## 1337	97	G97A	0.7936687571	1
## 1338	97	G97P	0.9526679587	1
## 1339	97	G97K	0.9403821716	1
## 1340	97	G97R	0.8606878342	1
## 1341	97	G97E	0.6404686610	1
## 1342	97	G97N	0.7672619405	1
## 1343	97	G97Q	1.2471605346	1
## 1344	97	G97Y	0.6219592985	1
## 1345	97	G97W	0.5942608452	0
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## 1347	97	G97I	0.5256966379	0
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## 1349	97	G97T	0.7809639599	1
## 1350	97	G97F	1.1493827944	1
## 1351	97	G97V	0.8545502050	1
## 1352	98	Q98H	0.3942903299	0
## 1353	98	Q98I	0.9939394761	1
## 1354	98	Q98L	0.7528405937	1
## 1355	98	Q98M	0.8630984664	1
## 1356	98	Q98N	1.0277478917	1
## 1357	98	Q98K	0.9062448523	1
## 1358	98	Q98W	0.6885954216	1

## 1359	98	Q98Y	0.8778453743	1
## 1360	98	Q98G	1.1392497870	1
## 1361	98	Q98T	0.9101820589	1
## 1362	98	Q98P	0.9098253492	1
## 1363	98	Q98R	0.8112847370	1
## 1364	98	Q98S	0.7007181768	1
## 1365	98	Q98V	0.9267674744	1
## 1366	98	Q98E	0.9252866913	1
## 1367	98	Q98F	0.6326593296	1
## 1368	98	Q98A	1.0761796768	1
## 1369	98	Q98C	0.8979651226	1
## 1370	98	Q98D	0.9820461134	1
## 1371	99	W99A	0.8553103286	1
## 1372	99	W99C	0.7214975315	1
## 1373	99	W99D	0.6931693174	1
## 1374	99	W99E	0.6598207800	1
## 1375	99	W99F	0.9196527120	1
## 1376	99	W99G	0.9257316369	1
## 1377	99	W99H	1.4032577668	1
## 1378	99	W99I	0.8700803854	1
## 1379	99	W99K	0.9487387207	1
## 1380	99	W99L	0.7955076827	1
## 1381	99	W99M	0.8553899366	1
## 1382	99	W99N	0.7262753148	1
## 1383	99	W99P	0.7885181619	1
## 1384	99	W99Q	0.8013073707	1
## 1385	99	W99R	0.8425729140	1
## 1386	99	W99S	0.9687317048	1
## 1387	99	W99T	0.9878676281	1
## 1388	99	W99V	0.9378538932	1
## 1389	99	W99Y	0.7239547246	1
## 1390	100	S100A	0.8900703260	1
## 1391	100	S100C	1.0614151503	1
## 1392	100	S100D	0.9691436688	1
## 1393	100	S100E	0.8026572686	1
## 1394	100	S100F	0.7062999863	1
## 1395	100	S100G	1.0525863800	1
## 1396	100	S100H	0.8999347057	1
## 1397	100	S100K	0.9177562542	1
## 1398	100	S100L	0.8623802713	1
## 1399	100	S100M	0.9094672397	1
## 1400	100	S100N	0.8891512751	1
## 1401	100	S100P	0.6771687064	1
## 1402	100	S100Q	1.1105244769	1
## 1403	100	S100R	0.9783195745	1
## 1404	100	S100T	0.7834204221	1
## 1405	100	S100V	1.0879209424	1
## 1406	100	S100Y	0.3654790738	0
## 1407	101	V101A	0.5765209644	0
## 1408	101	V101C	0.7872532663	1
## 1409	101	V101D	0.8826743905	1
## 1410	101	V101E	1.0448402862	1
## 1411	101	V101F	0.6927837397	1
## 1412	101	V101G	0.6936813377	1

## 1413	101	V101H	0.8828802499	1
## 1414	101	V101I	1.1378587722	1
## 1415	101	V101K	0.8818339970	1
## 1416	101	V101L	1.2381049394	1
## 1417	101	V101M	0.7877039977	1
## 1418	101	V101N	0.4480069169	0
## 1419	101	V101P	0.5534561722	0
## 1420	101	V101Q	0.7705275743	1
## 1421	101	V101R	0.7226633406	1
## 1422	101	V101S	0.4983974608	0
## 1423	101	V101T	0.7576135599	1
## 1424	101	V101W	0.8162634669	1
## 1425	101	V101Y	0.5885726332	0
## 1426	102	K102F	1.0365365680	1
## 1427	102	K102D	0.8319271412	1
## 1428	102	K102E	0.9924382394	1
## 1429	102	K102S	0.6435227828	1
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## 1431	102	K102C	0.7762082178	1
## 1432	102	K102A	0.7623852915	1
## 1433	102	K102T	0.6814126711	1
## 1434	102	K102V	0.7379239047	1
## 1435	102	K102Y	0.8246294629	1
## 1436	102	K102W	0.8845482910	1
## 1437	102	K102R	0.8063341768	1
## 1438	102	K102H	0.4531100092	0
## 1439	102	K102I	0.9933129980	1
## 1440	102	K102Q	1.1840709613	1
## 1441	102	K102P	0.0060975053	0
## 1442	102	K102L	0.6731264121	1
## 1443	103	T103A	0.9592061690	1
## 1444	103	T103C	1.0377178953	1
## 1445	103	T103D	0.4043323923	0
## 1446	103	T103E	0.7974040494	1
## 1447	103	T103F	0.7798734613	1
## 1448	103	T103G	0.6856619318	1
## 1449	103	T103H	1.0013494757	1
## 1450	103	T103I	0.6571906689	1
## 1451	103	T103K	0.7965639241	1
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## 1465	104	K104W	0.8177765707	1
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## 1474	104	K104C	0.4769392503	0
## 1475	104	K104Q	1.0208229914	1
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## 1477	104	K104Y	0.7155513541	1
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## 1481	105	H105I	1.0548537726	1
## 1482	105	H105M	0.1226098737	0
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## 1488	105	H105Q	0.5762627092	0
## 1489	105	H105N	-0.0360870886	0
## 1490	105	H105G	0.7045654630	1
## 1491	105	H105A	0.6201983267	1
## 1492	105	H105R	1.0111896830	1
## 1493	105	H105L	0.8289692190	1
## 1494	105	H105S	0.7601799318	1
## 1495	105	H105F	0.9007422437	1
## 1496	105	H105W	0.8953894670	1
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## 1499	105	H105T	1.0847146265	1
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## 1501	106	Q106R	0.9330648653	1
## 1502	106	Q106V	1.1108052927	1
## 1503	106	Q106W	0.5940670340	0
## 1504	106	Q106S	0.9039754585	1
## 1505	106	Q106T	1.0004339684	1
## 1506	106	Q106E	0.9932088658	1
## 1507	106	Q106F	0.8491109257	1
## 1508	106	Q106A	0.8152251287	1
## 1509	106	Q106C	0.9435083754	1
## 1510	106	Q106M	0.8921847398	1
## 1511	106	Q106N	1.0689375051	1
## 1512	106	Q106P	0.1918743792	0
## 1513	106	Q106G	0.8127429987	1
## 1514	106	Q106K	0.9662159668	1
## 1515	106	Q106L	0.9234858733	1
## 1516	106	Q106I	1.1142547133	1
## 1517	106	Q106H	0.6664675672	1
## 1518	107	M107V	0.9118217758	1
## 1519	107	M107T	0.8890192482	1
## 1520	107	M107W	0.8252968358	1

## 1521	107	M107Y	0.9740960810	1
## 1522	107	M107E	1.1189139973	1
## 1523	107	M107A	1.0429908040	1
## 1524	107	M107C	0.7215039717	1
## 1525	107	M107D	1.1209908268	1
## 1526	107	M107R	1.0038665956	1
## 1527	107	M107S	1.0249792725	1
## 1528	107	M107P	0.6375212733	1
## 1529	107	M107N	1.0073415528	1
## 1530	107	M107Q	1.0658603020	1
## 1531	107	M107G	1.0879787216	1
## 1532	107	M107H	0.8377781276	1
## 1533	107	M107I	0.8312186781	1
## 1534	107	M107F	1.0336043121	1
## 1535	107	M107L	0.8986707227	1
## 1536	107	M107K	1.2013481544	1
## 1537	108	Y108A	0.3624312904	0
## 1538	108	Y108C	0.7020618701	1
## 1539	108	Y108D	0.2297596081	0
## 1540	108	Y108E	0.3586525143	0
## 1541	108	Y108F	1.1804088135	1
## 1542	108	Y108G	0.2779934167	0
## 1543	108	Y108H	0.4891838834	0
## 1544	108	Y108I	0.8286498613	1
## 1545	108	Y108K	0.6741228211	1
## 1546	108	Y108L	-0.0203356092	0
## 1547	108	Y108M	0.1783682562	0
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## 1549	108	Y108P	-0.0155087543	0
## 1550	108	Y108Q	0.3190125904	0
## 1551	108	Y108R	0.2551517437	0
## 1552	108	Y108S	0.2686544326	0
## 1553	108	Y108T	0.1084168907	0
## 1554	108	Y108V	0.5337699823	0
## 1555	108	Y108W	1.0156914332	1
## 1556	109	S109A	0.9667442203	1
## 1557	109	S109C	0.8386904375	1
## 1558	109	S109D	1.2827543669	1
## 1559	109	S109E	1.2113177691	1
## 1560	109	S109F	0.5506449539	0
## 1561	109	S109G	0.8196444598	1
## 1562	109	S109H	0.8448504501	1
## 1563	109	S109I	0.6615593911	1
## 1564	109	S109K	1.1551458991	1
## 1565	109	S109L	0.9363760824	1
## 1566	109	S109M	1.0329558898	1
## 1567	109	S109N	0.9814742682	1
## 1568	109	S109P	1.3809250315	1
## 1569	109	S109Q	0.9730983795	1
## 1570	109	S109R	1.1096164860	1
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## 1572	109	S109V	0.9504572781	1
## 1573	109	S109W	0.7872205409	1
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## 1576	110	I110Q	0.6512397323	1
## 1577	110	I110D	-0.2693114072	0
## 1578	110	I110N	-0.1028761384	0
## 1579	110	I110P	0.5863043803	0
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## 1581	110	I110M	0.9665191882	1
## 1582	110	I110S	0.3462416748	0
## 1583	110	I110L	0.9773401874	1
## 1584	110	I110W	0.6990255873	1
## 1585	110	I110R	0.3620194962	0
## 1586	110	I110Y	0.6273930687	1
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## 1588	110	I110F	0.7936422654	1
## 1589	110	I110A	0.1896483599	0
## 1590	110	I110K	-0.2372629436	0
## 1591	110	I110H	-0.0760705426	0
## 1592	110	I110G	0.1325802561	0
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## 1594	111	P111Y	0.6443926098	1
## 1595	111	P111S	0.9201359450	1
## 1596	111	P111T	1.1510599581	1
## 1597	111	P111W	0.5221603574	0
## 1598	111	P111R	0.8828738390	1
## 1599	111	P111C	0.6493397284	1
## 1600	111	P111D	0.8541501208	1
## 1601	111	P111V	0.1679112507	0
## 1602	111	P111A	0.8222184983	1
## 1603	111	P111H	0.9915786373	1
## 1604	111	P111L	0.4295509693	0
## 1605	111	P111M	0.6788351989	1
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## 1607	111	P111Q	0.4491885852	0
## 1608	111	P111G	0.8546374491	1
## 1609	111	P111I	0.3210872886	0
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## 1611	111	P111F	0.2725935779	0
## 1612	111	P111K	1.2156735065	1
## 1613	112	E112Y	0.8477959126	1
## 1614	112	E112T	0.8340281398	1
## 1615	112	E112G	0.9391369699	1
## 1616	112	E112W	0.5270532873	0
## 1617	112	E112C	0.7844334779	1
## 1618	112	E112F	0.9001934340	1
## 1619	112	E112A	0.8021290182	1
## 1620	112	E112D	0.5897616520	0
## 1621	112	E112V	0.8986544191	1
## 1622	112	E112R	0.7790393456	1
## 1623	112	E112H	0.9985531324	1
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## 1625	112	E112M	0.7623937417	1
## 1626	112	E112S	0.8195362969	1
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## 1629	112	E112K	1.2214253398	1
## 1630	112	E112P	0.7823247056	1
## 1631	112	E112L	0.8065149106	1
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## 1633	113	D113M	0.7675725788	1
## 1634	113	D113G	1.0821664043	1
## 1635	113	D113W	1.0367594703	1
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## 1642	113	D113K	0.8845844645	1
## 1643	113	D113I	0.9867152855	1
## 1644	113	D113Y	1.0191465923	1
## 1645	113	D113E	0.9978091686	1
## 1646	113	D113A	0.9906846023	1
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## 1659	114	A114M	1.1746042394	1
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## 1663	114	A114G	0.8390628571	1
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## 1669	115	M115P	0.4908625820	0
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## 1671	115	M115S	1.0145508376	1
## 1672	115	M115N	0.8032887683	1
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## 1675	115	M115L	1.0893449826	1
## 1676	115	M115Y	0.8299831969	1
## 1677	115	M115F	0.9599619308	1
## 1678	115	M115G	0.9754966870	1
## 1679	115	M115C	1.0377374743	1
## 1680	115	M115D	0.7915779547	1
## 1681	115	M115W	0.9105255410	1
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## 1684	115 M115I	0.7405795682	1
## 1685	115 M115V	0.8231372752	1
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## 1687	116 T116A	1.1442155816	1
## 1688	116 T116C	1.0684759219	1
## 1689	116 T116D	1.1781522282	1
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## 1691	116 T116G	1.0398702376	1
## 1692	116 T116H	0.6837822352	1
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## 1712	117 G117S	0.7055114107	1
## 1713	117 G117C	0.1050384023	0
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## 1718	117 G117W	0.8153877770	1
## 1719	117 G117Q	0.7037078335	1
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## 1754	119	A119D	0.7894297912	1
## 1755	119	A119M	0.9362967384	1
## 1756	119	A119E	0.9529704117	1
## 1757	119	A119S	0.8345699664	1
## 1758	119	A119F	1.0284161370	1
## 1759	119	A119W	0.6674355327	1
## 1760	119	A119C	0.9885216732	1
## 1761	120	E120H	0.6358396103	1
## 1762	120	E120A	0.5904017260	0
## 1763	120	E120W	0.7502406024	1
## 1764	120	E120V	0.9144333199	1
## 1765	120	E120N	0.6101101639	1
## 1766	120	E120P	0.7501795941	1
## 1767	120	E120L	0.5876528126	0
## 1768	120	E120Y	1.1473484323	1
## 1769	120	E120M	0.5092310534	0
## 1770	120	E120D	1.1270240618	1
## 1771	120	E120I	0.5655070287	0
## 1772	120	E120K	-0.4030756514	0
## 1773	120	E120G	0.8451203653	1
## 1774	120	E120T	0.2160892121	0
## 1775	120	E120S	0.6098698621	1
## 1776	120	E120Q	0.1303812505	0
## 1777	120	E120C	0.9538112584	1
## 1778	120	E120F	0.7282308641	1
## 1779	120	E120R	0.7739745673	1
## 1780	121	M121Y	0.6814563090	1
## 1781	121	M121V	1.1256798360	1
## 1782	121	M121W	0.8086579192	1
## 1783	121	M121S	1.1272075866	1
## 1784	121	M121T	1.0558740015	1
## 1785	121	M121F	0.8384414035	1
## 1786	121	M121R	1.0439806982	1
## 1787	121	M121G	0.8997060994	1
## 1788	121	M121C	1.0463190816	1
## 1789	121	M121E	0.8709476152	1
## 1790	121	M121P	0.5355264026	0

## 1791	121	M121A	1.0670964348	1
## 1792	121	M121I	0.8840649948	1
## 1793	121	M121D	1.0204662325	1
## 1794	121	M121Q	0.7807641455	1
## 1795	121	M121H	0.5472818330	0
## 1796	121	M121K	0.6583450516	1
## 1797	121	M121L	0.8053780020	1
## 1798	121	M121N	0.7906033352	1
## 1799	122	L122R	0.5738730854	0
## 1800	122	L122S	0.6725924699	1
## 1801	122	L122C	0.6388204173	1
## 1802	122	L122T	0.5041795981	0
## 1803	122	L122G	0.8379862413	1
## 1804	122	L122D	0.5759169152	0
## 1805	122	L122Q	0.6764057937	1
## 1806	122	L122H	0.8485155024	1
## 1807	122	L122A	0.9089853778	1
## 1808	122	L122I	0.8117075716	1
## 1809	122	L122E	0.7248633072	1
## 1810	122	L122F	0.9483102923	1
## 1811	122	L122W	0.7475390224	1
## 1812	122	L122Y	1.3649245110	1
## 1813	122	L122V	1.1464249992	1
## 1814	122	L122N	0.6555183346	1
## 1815	122	L122P	0.4477805415	0
## 1816	122	L122K	1.1155829693	1
## 1817	123	F123E	0.5967955030	0
## 1818	123	F123N	0.5987546901	0
## 1819	123	F123D	0.6955616791	1
## 1820	123	F123H	0.2353146282	0
## 1821	123	F123S	0.7789960072	1
## 1822	123	F123T	0.3235406043	0
## 1823	123	F123G	0.8933353622	1
## 1824	123	F123M	0.9870191014	1
## 1825	123	F123Q	-0.0461168851	0
## 1826	123	F123I	0.6464343554	1
## 1827	123	F123C	1.1506218033	1
## 1828	123	F123R	0.2144100906	0
## 1829	123	F123A	0.4276757623	0
## 1830	123	F123L	0.3799936313	0
## 1831	123	F123K	0.2408020347	0
## 1832	123	F123Y	0.8327934607	1
## 1833	123	F123W	0.8385576877	1
## 1834	123	F123P	0.0939648594	0
## 1835	123	F123V	0.8856691109	1
## 1836	124	D124Q	0.7261561063	1
## 1837	124	D124I	0.0209231430	0
## 1838	124	D124F	0.1795476109	0
## 1839	124	D124G	0.6220438734	1
## 1840	124	D124A	0.6154930421	1
## 1841	124	D124C	0.6154878260	1
## 1842	124	D124P	0.3437356458	0
## 1843	124	D124L	0.4930795202	0
## 1844	124	D124K	0.2110849841	0

## 1845	124	D124E	0.6888336413	1
## 1846	124	D124R	0.1955017143	0
## 1847	124	D124V	0.5343591427	0
## 1848	124	D124S	0.6510306887	1
## 1849	124	D124M	0.4393003394	0
## 1850	124	D124W	0.4083061374	0
## 1851	124	D124T	0.7602501141	1
## 1852	125	Y125A	0.6856563770	1
## 1853	125	Y125C	0.6719984020	1
## 1854	125	Y125D	0.2648341977	0
## 1855	125	Y125E	0.8766393567	1
## 1856	125	Y125F	1.1745212576	1
## 1857	125	Y125G	0.2998020818	0
## 1858	125	Y125H	0.7832751685	1
## 1859	125	Y125I	0.8248782247	1
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## 1861	125	Y125L	0.7329106740	1
## 1862	125	Y125M	0.5616944814	0
## 1863	125	Y125N	0.5524564172	0
## 1864	125	Y125P	0.3378696127	0
## 1865	125	Y125Q	1.0528526557	1
## 1866	125	Y125R	0.5643655210	0
## 1867	125	Y125S	0.8401458672	1
## 1868	125	Y125T	0.2521911855	0
## 1869	125	Y125V	0.8647376616	1
## 1870	125	Y125W	0.7759842205	1
## 1871	126	I126K	0.2154005256	0
## 1872	126	I126G	0.0983917602	0
## 1873	126	I126C	0.7890106778	1
## 1874	126	I126A	0.6119861199	1
## 1875	126	I126H	0.0714486613	0
## 1876	126	I126M	0.4078755827	0
## 1877	126	I126E	-0.2448073979	0
## 1878	126	I126D	-0.0528444469	0
## 1879	126	I126L	0.8302690510	1
## 1880	126	I126F	1.1669720363	1
## 1881	126	I126V	0.7264486232	1
## 1882	126	I126Y	0.3170129776	0
## 1883	126	I126W	0.2786156882	0
## 1884	126	I126N	0.1369885824	0
## 1885	126	I126P	-0.3633865065	0
## 1886	126	I126T	0.5863046975	0
## 1887	126	I126Q	0.1824797580	0
## 1888	126	I126S	-0.2645940738	0
## 1889	126	I126R	-0.1186288719	0
## 1890	127	S127A	0.8640394844	1
## 1891	127	S127C	1.0629324996	1
## 1892	127	S127D	-0.0973588140	0
## 1893	127	S127E	0.7628117443	1
## 1894	127	S127F	0.7557487603	1
## 1895	127	S127G	0.8440511246	1
## 1896	127	S127H	0.3230418478	0
## 1897	127	S127I	0.2333294809	0
## 1898	127	S127K	1.1871103163	1

## 1899	127	S127L	0.5648806100	0
## 1900	127	S127N	0.6741197709	1
## 1901	127	S127P	0.0146299166	0
## 1902	127	S127R	0.5047068158	0
## 1903	127	S127T	0.7628921352	1
## 1904	127	S127V	0.8482068420	1
## 1905	127	S127W	0.7696879589	1
## 1906	128	E128M	1.1029810033	1
## 1907	128	E128Y	0.7230221977	1
## 1908	128	E128L	0.8134434247	1
## 1909	128	E128K	1.0280138748	1
## 1910	128	E128G	0.8015867798	1
## 1911	128	E128H	0.3854275264	0
## 1912	128	E128W	0.5626193850	0
## 1913	128	E128F	0.8950892203	1
## 1914	128	E128A	0.5913662628	0
## 1915	128	E128N	0.2345050427	0
## 1916	128	E128I	1.1844557412	1
## 1917	128	E128V	0.8652444567	1
## 1918	128	E128C	0.7262044115	1
## 1919	128	E128S	0.7098863602	1
## 1920	128	E128R	0.7692525712	1
## 1921	128	E128P	0.2906578272	0
## 1922	128	E128T	1.1443185874	1
## 1923	128	E128Q	0.9394710781	1
## 1924	129	C129T	0.7109969034	1
## 1925	129	C129A	0.9921026572	1
## 1926	129	C129V	0.6814969560	1
## 1927	129	C129K	0.9094892859	1
## 1928	129	C129L	0.3188242193	0
## 1929	129	C129I	0.6294108772	1
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## 1931	129	C129N	0.4035186408	0
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## 1933	129	C129M	0.5238476660	0
## 1934	129	C129D	0.5962829114	0
## 1935	129	C129W	0.6732867564	1
## 1936	129	C129Q	0.0348379064	0
## 1937	129	C129E	0.9591150711	1
## 1938	129	C129H	0.5529045097	0
## 1939	129	C129R	0.5074929356	0
## 1940	129	C129G	0.7832939804	1
## 1941	130	I130E	0.1194550122	0
## 1942	130	I130F	0.4800362237	0
## 1943	130	I130T	0.4818756524	0
## 1944	130	I130G	0.0263885538	0
## 1945	130	I130C	0.7521144537	1
## 1946	130	I130R	0.0027008440	0
## 1947	130	I130S	0.1955796207	0
## 1948	130	I130K	-0.1888846952	0
## 1949	130	I130V	0.8549208268	1
## 1950	130	I130W	0.5153872452	0
## 1951	130	I130H	-0.1309081275	0
## 1952	130	I130Y	0.3564149884	0

## 1953	130	I130L	0.8462050200	1
## 1954	130	I130Q	0.3511265304	0
## 1955	130	I130N	-0.3194802071	0
## 1956	130	I130A	0.6635294834	1
## 1957	130	I130P	-0.1051429208	0
## 1958	131	S131A	0.9403303605	1
## 1959	131	S131C	0.9998370290	1
## 1960	131	S131D	0.9304817990	1
## 1961	131	S131E	1.3720365938	1
## 1962	131	S131F	0.7027295584	1
## 1963	131	S131G	1.0295150038	1
## 1964	131	S131H	0.8294132806	1
## 1965	131	S131I	0.6239776348	1
## 1966	131	S131K	0.9186318319	1
## 1967	131	S131L	0.8791004135	1
## 1968	131	S131M	0.3600644126	0
## 1969	131	S131N	1.0947000090	1
## 1970	131	S131P	0.1822612005	0
## 1971	131	S131Q	0.4020769513	0
## 1972	131	S131R	1.0131393575	1
## 1973	131	S131T	0.6533426674	1
## 1974	131	S131V	1.1284001616	1
## 1975	131	S131W	0.6945142218	1
## 1976	131	S131Y	0.7998567736	1
## 1977	132	D132S	0.6102153614	1
## 1978	132	D132T	0.5897756074	0
## 1979	132	D132V	0.8586437027	1
## 1980	132	D132M	1.1388252659	1
## 1981	132	D132G	1.0745612186	1
## 1982	132	D132F	0.8170551807	1
## 1983	132	D132R	0.6344833120	1
## 1984	132	D132P	-0.0960511980	0
## 1985	132	D132I	0.9909198765	1
## 1986	132	D132E	0.6907126032	1
## 1987	132	D132C	0.7705558893	1
## 1988	132	D132W	0.7200447846	1
## 1989	132	D132L	0.9036938751	1
## 1990	132	D132Y	0.4436350404	0
## 1991	132	D132Q	0.5810756442	0
## 1992	132	D132N	0.7451032767	1
## 1993	132	D132H	0.7481504792	1
## 1994	132	D132A	0.9223917199	1
## 1995	132	D132K	0.9839619322	1
## 1996	133	F133K	0.0021994724	0
## 1997	133	F133Q	0.3433200758	0
## 1998	133	F133E	0.3918328026	0
## 1999	133	F133D	-0.0450694042	0
## 2000	133	F133C	0.3405149695	0
## 2001	133	F133I	0.4025394178	0
## 2002	133	F133P	0.2062158158	0
## 2003	133	F133M	0.9017678334	1
## 2004	133	F133R	0.2018922405	0
## 2005	133	F133H	0.4401301527	0
## 2006	133	F133G	-0.0052788782	0

## 2007	133	F133V	0.2496187176	0
## 2008	133	F133A	0.4042225285	0
## 2009	133	F133L	0.5756839436	0
## 2010	133	F133N	0.3107758368	0
## 2011	133	F133Y	0.7213381722	1
## 2012	133	F133T	0.5964924467	0
## 2013	133	F133W	0.4020752984	0
## 2014	133	F133S	0.2746764146	0
## 2015	134	L134I	0.9434488055	1
## 2016	134	L134N	0.7326375493	1
## 2017	134	L134G	0.2430379672	0
## 2018	134	L134H	0.3778256956	0
## 2019	134	L134S	0.5178076094	0
## 2020	134	L134C	0.9366113295	1
## 2021	134	L134Y	0.5198111629	0
## 2022	134	L134W	0.6977667771	1
## 2023	134	L134R	0.5776487420	0
## 2024	134	L134V	0.8930556152	1
## 2025	134	L134K	0.3976392059	0
## 2026	134	L134Q	0.4500969391	0
## 2027	134	L134A	0.8467050935	1
## 2028	134	L134P	-0.0806472534	0
## 2029	134	L134E	0.5624317365	0
## 2030	134	L134T	0.4395426298	0
## 2031	134	L134D	0.0820214631	0
## 2032	135	D135W	0.4483451390	0
## 2033	135	D135V	1.0072498639	1
## 2034	135	D135I	0.9014852506	1
## 2035	135	D135L	0.6254946980	1
## 2036	135	D135S	0.9341584013	1
## 2037	135	D135M	0.8015565183	1
## 2038	135	D135G	0.9203923967	1
## 2039	135	D135F	0.5703143896	0
## 2040	135	D135T	0.9148451083	1
## 2041	135	D135A	0.9142394322	1
## 2042	135	D135H	0.6230649833	1
## 2043	135	D135E	0.9497160220	1
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## 2050	136	K136H	0.5983591818	0
## 2051	136	K136Y	0.7024172029	1
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## 2054	136	K136T	0.6996534876	1
## 2055	136	K136F	0.8093281000	1
## 2056	136	K136C	0.9170037234	1
## 2057	136	K136W	0.5271072929	0
## 2058	136	K136A	0.7205481793	1
## 2059	136	K136M	0.7202234002	1
## 2060	136	K136R	0.9816173768	1

## 2061	136	K136D	0.9734813772	1
## 2062	136	K136L	0.8994453568	1
## 2063	136	K136E	0.6814359800	1
## 2064	136	K136I	0.8483768094	1
## 2065	136	K136Q	0.6176109823	1
## 2066	136	K136P	-0.0110803156	0
## 2067	137	H137F	0.6768310775	1
## 2068	137	H137P	0.1462039181	0
## 2069	137	H137Q	0.8864729631	1
## 2070	137	H137G	0.5690925789	0
## 2071	137	H137E	0.7799505883	1
## 2072	137	H137T	0.5251949013	0
## 2073	137	H137I	0.5405971204	0
## 2074	137	H137R	0.7705286532	1
## 2075	137	H137S	0.8452046754	1
## 2076	137	H137N	-0.2098890400	0
## 2077	137	H137A	0.8418907622	1
## 2078	137	H137V	0.8370106311	1
## 2079	137	H137D	0.4373795871	0
## 2080	137	H137M	0.8968759800	1
## 2081	137	H137W	0.7623497614	1
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## 2085	137	H137L	0.8406798544	1
## 2086	138	Q138L	0.7135124052	1
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## 2100	138	Q138S	0.9000601980	1
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## 2102	138	Q138V	0.6971106622	1
## 2103	138	Q138G	0.9475970993	1
## 2104	139	M139C	0.8907804051	1
## 2105	139	M139A	0.8511930426	1
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## 2124	140	K140T	0.9232339392	1
## 2125	140	K140G	0.6334785930	1
## 2126	140	K140A	1.0254018143	1
## 2127	140	K140L	1.0118323468	1
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## 2129	140	K140W	0.7683970750	1
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## 2154	141	H141A	0.8725732025	1
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## 2163	142	K142V	0.9919263120	1
## 2164	142	K142N	0.5621673818	0
## 2165	142	K142L	0.8806041255	1
## 2166	142	K142S	0.8730509082	1
## 2167	142	K142P	0.6707506340	1
## 2168	142	K142A	0.8120332823	1

## 2169	142	K142R	0.8851424171	1
## 2170	142	K142C	0.9613164444	1
## 2171	142	K142E	0.9756442649	1
## 2172	142	K142Q	1.3240320575	1
## 2173	142	K142I	0.9255073992	1
## 2174	142	K142D	0.5923767228	0
## 2175	142	K142G	0.7723870681	1
## 2176	142	K142H	0.8673260492	1
## 2177	142	K142F	0.7867904103	1
## 2178	143	K143P	0.6258397398	1
## 2179	143	K143N	0.8418290097	1
## 2180	143	K143F	0.6417962304	1
## 2181	143	K143A	0.5019301796	0
## 2182	143	K143Q	1.0298824029	1
## 2183	143	K143Y	0.5904049108	0
## 2184	143	K143D	0.5103046439	0
## 2185	143	K143G	0.8703490122	1
## 2186	143	K143W	0.7508045411	1
## 2187	143	K143C	1.0061928885	1
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## 2189	143	K143E	0.7805765963	1
## 2190	143	K143T	1.0680953337	1
## 2191	143	K143M	0.7821798119	1
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## 2194	143	K143S	0.6986779340	1
## 2195	143	K143L	0.8289432516	1
## 2196	143	K143I	0.7825457119	1
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## 2198	144	L144T	0.5217362432	0
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## 2200	144	L144K	-0.1401559613	0
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## 2203	144	L144N	-0.0039488236	0
## 2204	144	L144A	0.3087919434	0
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## 2207	144	L144P	0.4809026298	0
## 2208	144	L144H	0.2397222284	0
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## 2211	144	L144V	0.9828547373	1
## 2212	144	L144Q	0.3684153206	0
## 2213	144	L144E	0.0864043253	0
## 2214	144	L144F	0.5172039120	0
## 2215	145	P145L	0.6233216333	1
## 2216	145	P145M	0.7254972436	1
## 2217	145	P145Q	0.3628793249	0
## 2218	145	P145R	0.6812893333	1
## 2219	145	P145A	0.5939259618	0
## 2220	145	P145N	0.8555633766	1
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## 2225	145	P145C	0.8086380286	1
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## 2228	145	P145F	0.5185801253	0
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## 2239	146	L146Q	0.3020493962	0
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## 2246	146	L146V	1.1170558506	1
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## 2248	146	L146T	1.0410066229	1
## 2249	146	L146A	0.8200142051	1
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## 2253	147	G147F	0.7570745839	1
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## 2257	147	G147A	0.8925493301	1
## 2258	147	G147D	0.3279948543	0
## 2259	147	G147V	0.7907804546	1
## 2260	147	G147S	0.8964240733	1
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## 2269	148	F148G	0.5531808417	0
## 2270	148	F148M	0.7178261190	1
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## 2276	148	F148P	0.1971240110	0

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## 2282	148	F148T	0.6895163954	1
## 2283	148	F148L	0.9462730986	1
## 2284	148	F148V	1.0617664611	1
## 2285	148	F148A	0.9907277294	1
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## 2287	149	T149C	1.1292942098	1
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## 2290	149	T149F	0.7254126360	1
## 2291	149	T149G	0.7905485806	1
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## 2293	149	T149I	0.7605551315	1
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## 2295	149	T149L	0.7677139884	1
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## 2302	149	T149V	1.1707158647	1
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## 2308	150	F150Q	0.8406447914	1
## 2309	150	F150I	0.7349955313	1
## 2310	150	F150P	0.7648917460	1
## 2311	150	F150V	1.0518222819	1
## 2312	150	F150W	1.0146555266	1
## 2313	150	F150M	0.9989632236	1
## 2314	150	F150K	1.3339226713	1
## 2315	150	F150L	1.0887817418	1
## 2316	150	F150G	1.1747788620	1
## 2317	150	F150R	0.9416022717	1
## 2318	150	F150D	0.8397208241	1
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## 2357	181	V181Y	0.8830540832	1
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## 2416	185	L185T	0.7322648167	1
## 2417	185	L185R	0.1752500496	0
## 2418	185	L185K	0.6000715280	1
## 2419	185	L185W	0.5119254116	0
## 2420	185	L185I	0.9033922748	1
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## 2436	186	R186M	1.0877036103	1
## 2437	186	R186F	0.6058948104	1
## 2438	186	R186G	0.8906333450	1

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## 2456	187	D187T	0.5339749661	0
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## 2491	189	I189D	0.6685532869	1
## 2492	189	I189M	0.9916610924	1

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## 2561	193	G193A	0.9552260835	1
## 2562	193	G193W	0.4198747089	0
## 2563	193	G193N	0.4596211025	0
## 2564	193	G193M	0.6964229780	1
## 2565	193	G193R	0.8128442221	1
## 2566	193	G193K	0.7816106592	1
## 2567	193	G193E	0.9923003615	1
## 2568	193	G193L	0.6288394078	1
## 2569	193	G193I	0.8639385599	1
## 2570	193	G193Q	1.0159948114	1
## 2571	193	G193H	0.6614299392	1
## 2572	193	G193F	0.6088646124	1
## 2573	193	G193Y	0.2263452432	0
## 2574	194	D194M	1.0455572536	1
## 2575	194	D194Q	1.0798601792	1
## 2576	194	D194T	0.6173386114	1
## 2577	194	D194N	1.0226560803	1
## 2578	194	D194K	0.9368250381	1
## 2579	194	D194L	1.2003452424	1
## 2580	194	D194F	1.0547109694	1
## 2581	194	D194V	0.8480977200	1
## 2582	194	D194R	0.3119020570	0
## 2583	194	D194G	0.8265850227	1
## 2584	194	D194S	0.7825838342	1
## 2585	194	D194E	0.7650866395	1
## 2586	194	D194W	0.7381605836	1
## 2587	194	D194Y	0.5753081075	0
## 2588	194	D194I	0.7147255366	1
## 2589	194	D194C	1.0270728983	1
## 2590	194	D194P	0.7617937692	1
## 2591	194	D194H	0.6610834344	1
## 2592	194	D194A	0.8834532350	1
## 2593	195	F195V	0.8149411912	1
## 2594	195	F195N	0.4141922928	0
## 2595	195	F195K	0.9174926670	1
## 2596	195	F195P	0.8507687136	1
## 2597	195	F195S	0.7937657153	1
## 2598	195	F195Q	0.7913012853	1
## 2599	195	F195R	0.6848597187	1
## 2600	195	F195I	0.6583185626	1

## 2601	195	F195T	0.8408394111	1
## 2602	195	F195H	1.2479478605	1
## 2603	195	F195A	0.9323849606	1
## 2604	195	F195D	0.9463665037	1
## 2605	195	F195L	0.9334448687	1
## 2606	195	F195M	0.9593299142	1
## 2607	195	F195W	1.1035475617	1
## 2608	195	F195E	0.9067838966	1
## 2609	195	F195G	0.9535815087	1
## 2610	195	F195Y	1.2562483216	1
## 2611	196	E196P	0.8152111872	1
## 2612	196	E196L	0.9586121634	1
## 2613	196	E196N	0.6084338401	1
## 2614	196	E196I	0.8358577679	1
## 2615	196	E196Y	0.7854857512	1
## 2616	196	E196R	0.8675793557	1
## 2617	196	E196S	1.0713432335	1
## 2618	196	E196Q	0.7411448444	1
## 2619	196	E196G	0.7358668217	1
## 2620	196	E196W	0.5463799104	0
## 2621	196	E196F	0.8453197060	1
## 2622	196	E196T	0.8259433970	1
## 2623	196	E196M	0.9479040710	1
## 2624	196	E196H	0.4733096158	0
## 2625	196	E196C	0.7723249291	1
## 2626	196	E196A	0.8039923018	1
## 2627	196	E196V	0.8476467959	1
## 2628	197	M197L	0.8960628429	1
## 2629	197	M197N	0.5195249804	0
## 2630	197	M197G	0.9782974327	1
## 2631	197	M197I	0.8211569822	1
## 2632	197	M197E	0.6523811171	1
## 2633	197	M197D	0.8515553863	1
## 2634	197	M197H	0.9814898232	1
## 2635	197	M197Q	0.9279569997	1
## 2636	197	M197T	1.1087128538	1
## 2637	197	M197Y	0.9049219809	1
## 2638	197	M197P	0.9821245611	1
## 2639	197	M197A	0.7524974093	1
## 2640	197	M197S	0.8126724448	1
## 2641	197	M197W	0.8321545475	1
## 2642	197	M197R	0.8421625427	1
## 2643	197	M197V	0.8989159406	1
## 2644	198	D198H	0.8735781538	1
## 2645	198	D198Q	0.7773290208	1
## 2646	198	D198R	0.5182580270	0
## 2647	198	D198G	0.8301773862	1
## 2648	198	D198F	0.5620324809	0
## 2649	198	D198L	0.4277032597	0
## 2650	198	D198K	0.4156717766	0
## 2651	198	D198S	1.0942272196	1
## 2652	198	D198E	1.0626172776	1
## 2653	198	D198W	0.4751088344	0
## 2654	198	D198T	0.5313788696	0

## 2655	198	D198M	0.4632187014	0
## 2656	198	D198P	0.9551003077	1
## 2657	198	D198V	0.4280337699	0
## 2658	198	D198I	-0.0054267065	0
## 2659	198	D198A	0.7556463015	1
## 2660	198	D198N	1.0944322110	1
## 2661	198	D198C	0.4663211499	0
## 2662	199	V199A	0.9887467061	1
## 2663	199	V199C	1.1063209003	1
## 2664	199	V199E	1.0801749454	1
## 2665	199	V199G	0.8458124132	1
## 2666	199	V199H	0.9012438057	1
## 2667	199	V199I	0.7067053271	1
## 2668	199	V199K	0.7311609936	1
## 2669	199	V199L	0.9406894259	1
## 2670	199	V199M	0.9769377448	1
## 2671	199	V199N	0.8186731695	1
## 2672	199	V199P	0.9189163138	1
## 2673	199	V199Q	1.1430902832	1
## 2674	199	V199R	0.7905044463	1
## 2675	199	V199S	1.0702954246	1
## 2676	199	V199T	1.1583190972	1
## 2677	199	V199W	0.8561430110	1
## 2678	199	V199Y	0.8778875582	1
## 2679	200	V200A	0.8187013660	1
## 2680	200	V200C	0.8361827421	1
## 2681	200	V200E	0.6795535231	1
## 2682	200	V200F	0.9794688442	1
## 2683	200	V200G	0.9128680024	1
## 2684	200	V200H	0.8054546017	1
## 2685	200	V200I	0.9222472870	1
## 2686	200	V200K	0.9860289805	1
## 2687	200	V200L	0.8260744269	1
## 2688	200	V200M	0.8572227887	1
## 2689	200	V200N	0.6535558211	1
## 2690	200	V200P	0.5997425030	0
## 2691	200	V200Q	0.6960959887	1
## 2692	200	V200R	0.7646065229	1
## 2693	200	V200S	0.4880193571	0
## 2694	200	V200T	0.9967781986	1
## 2695	200	V200W	1.0484229611	1
## 2696	200	V200Y	0.9929580152	1
## 2697	201	A201T	-0.0166302362	0
## 2698	201	A201Q	0.7178603185	1
## 2699	201	A201Y	0.4057716542	0
## 2700	201	A201R	0.8010022626	1
## 2701	201	A201L	0.8063453472	1
## 2702	201	A201H	0.5118481497	0
##	ESM.1v	DMS_score_activity	DMS_score_bin_activity	V1 Model
## 1	-8.11408691	0.929542509	1	264 ThermoMPNN
## 2	-4.88893480	1.186318685	1	268 ThermoMPNN
## 3	-6.10889454	0.693208860	1	271 ThermoMPNN
## 4	-4.80996170	1.221512028	1	262 ThermoMPNN
## 5	-4.65416546	1.333086826	1	274 ThermoMPNN

## 6	-4.37980862	0.396535439	0	265	ThermoMPNN
## 7	-4.86078358	0.932691335	1	269	ThermoMPNN
## 8	-7.29920807	0.958929503	1	261	ThermoMPNN
## 9	-6.21627188	2.717458770	1	270	ThermoMPNN
## 10	-6.98746090	0.663562953	1	267	ThermoMPNN
## 11	-5.10519671	1.253651766	1	275	ThermoMPNN
## 12	-4.51215572	1.025237712	1	273	ThermoMPNN
## 13	-6.45480547	1.116282613	1	266	ThermoMPNN
## 14	-8.59858904	1.506047699	1	279	ThermoMPNN
## 15	-5.90419664	0.660073683	1	276	ThermoMPNN
## 16	-6.32254696	1.331429435	1	272	ThermoMPNN
## 17	-4.35083280	0.870904441	1	260	ThermoMPNN
## 18	-7.92981024	0.796932308	1	278	ThermoMPNN
## 19	-5.52361088	1.057761509	1	277	ThermoMPNN
## 20	-5.42510762	1.597320328	1	280	ThermoMPNN
## 21	-9.48956966	1.096085913	1	298	ThermoMPNN
## 22	-7.63281293	0.844157766	1	299	ThermoMPNN
## 23	-6.73013430	0.900288260	1	297	ThermoMPNN
## 24	-2.97539614	0.014787938	0	293	ThermoMPNN
## 25	-7.61840858	0.737161999	1	281	ThermoMPNN
## 26	-5.71867476	1.496681648	1	295	ThermoMPNN
## 27	-5.96811657	0.627688101	1	296	ThermoMPNN
## 28	-7.02677994	1.886167091	1	290	ThermoMPNN
## 29	-3.81374102	1.458114972	1	283	ThermoMPNN
## 30	-6.26173277	1.373991134	1	285	ThermoMPNN
## 31	-6.11256700	1.004091186	1	282	ThermoMPNN
## 32	-7.53113041	1.301635531	1	287	ThermoMPNN
## 33	-7.99820805	1.151093126	1	292	ThermoMPNN
## 34	-9.05664501	1.626957550	1	284	ThermoMPNN
## 35	-4.04828968	1.461861667	1	294	ThermoMPNN
## 36	-6.54482059	1.490204061	1	289	ThermoMPNN
## 37	-5.34840927	1.604686916	1	286	ThermoMPNN
## 38	-5.54116166	1.149890084	1	300	ThermoMPNN
## 39	-12.95642204	0.683029713	1	302	ThermoMPNN
## 40	-10.51368599	0.818051843	1	303	ThermoMPNN
## 41	-10.44321499	0.662261431	1	304	ThermoMPNN
## 42	-10.62793751	0.845166987	1	305	ThermoMPNN
## 43	-12.43289471	1.444143797	1	306	ThermoMPNN
## 44	-5.90850611	1.169338633	1	307	ThermoMPNN
## 45	-10.83213100	1.058033657	1	308	ThermoMPNN
## 46	-6.57301035	1.926277280	1	309	ThermoMPNN
## 47	-6.64927378	2.563323927	1	310	ThermoMPNN
## 48	-12.49390583	0.715412485	1	311	ThermoMPNN
## 49	-11.56001759	0.590205691	1	312	ThermoMPNN
## 50	-11.26305275	0.337736420	0	313	ThermoMPNN
## 51	-10.93657932	1.152623188	1	314	ThermoMPNN
## 52	-9.66963806	1.541270962	1	315	ThermoMPNN
## 53	-6.95146770	1.034768097	1	316	ThermoMPNN
## 54	-12.51078053	1.033718957	1	318	ThermoMPNN
## 55	-11.85532742	1.226384480	1	319	ThermoMPNN
## 56	-9.68199215	1.667770327	1	332	ThermoMPNN
## 57	-4.83602839	0.508583217	0	333	ThermoMPNN
## 58	-7.00882692	0.987309969	1	326	ThermoMPNN
## 59	-6.34577112	0.683433344	1	325	ThermoMPNN

## 60	-9.96752396	0.395006723	0	339	ThermoMPNN
## 61	-7.60830717	1.484972073	1	329	ThermoMPNN
## 62	-6.18336220	0.094976857	0	331	ThermoMPNN
## 63	-9.73823671	1.193156872	1	327	ThermoMPNN
## 64	-5.59506960	0.278066272	0	328	ThermoMPNN
## 65	-10.65890446	1.530000660	1	324	ThermoMPNN
## 66	-6.47269788	1.238060232	1	335	ThermoMPNN
## 67	-6.45247650	1.100034915	1	334	ThermoMPNN
## 68	-7.16821346	0.402639714	0	336	ThermoMPNN
## 69	-10.80969219	1.378086622	1	338	ThermoMPNN
## 70	-4.35738058	1.207317682	1	322	ThermoMPNN
## 71	-6.12209625	1.189016875	1	320	ThermoMPNN
## 72	-8.18332319	0.885351686	1	337	ThermoMPNN
## 73	-9.59451656	1.063536373	1	321	ThermoMPNN
## 74	-1.99546307	0.797900102	1	343	ThermoMPNN
## 75	-8.23233280	0.902642296	1	341	ThermoMPNN
## 76	-4.69683933	0.295479324	0	342	ThermoMPNN
## 77	-7.07727737	1.246675862	1	357	ThermoMPNN
## 78	-9.87043304	1.445486198	1	359	ThermoMPNN
## 79	-6.21354790	0.710180064	1	351	ThermoMPNN
## 80	-4.50454378	0.643238074	1	345	ThermoMPNN
## 81	-6.21113291	1.485011895	1	346	ThermoMPNN
## 82	-9.35917320	0.619083465	1	358	ThermoMPNN
## 83	-6.66590109	1.736028202	1	356	ThermoMPNN
## 84	-7.57438021	1.498290176	1	350	ThermoMPNN
## 85	-9.87182655	0.440454984	0	352	ThermoMPNN
## 86	-4.24519839	0.842546703	1	354	ThermoMPNN
## 87	-10.27010250	1.511455533	1	344	ThermoMPNN
## 88	-5.06446919	1.381046872	1	340	ThermoMPNN
## 89	-7.09954710	0.791339699	1	349	ThermoMPNN
## 90	-5.96062641	0.512660995	0	355	ThermoMPNN
## 91	-3.97535167	1.791727968	1	348	ThermoMPNN
## 92	-8.89579163	0.336871860	0	347	ThermoMPNN
## 93	-8.96140146	0.478558890	0	376	ThermoMPNN
## 94	-11.92592983	1.284534105	1	375	ThermoMPNN
## 95	-11.56582479	0.923012910	1	361	ThermoMPNN
## 96	-5.95364113	1.521144079	1	377	ThermoMPNN
## 97	-13.18411369	1.935495764	1	371	ThermoMPNN
## 98	-10.01836014	1.742828340	1	360	ThermoMPNN
## 99	-13.05918846	0.796833370	1	378	ThermoMPNN
## 100	-12.44009247	1.169360702	1	374	ThermoMPNN
## 101	-13.11652126	0.957988380	1	363	ThermoMPNN
## 102	-5.78035383	1.524274659	1	369	ThermoMPNN
## 103	-12.10480156	0.447296847	0	373	ThermoMPNN
## 104	-14.16172867	1.253249099	1	362	ThermoMPNN
## 105	-11.63783684	0.060471246	0	366	ThermoMPNN
## 106	-7.62189512	1.676685098	1	364	ThermoMPNN
## 107	-12.14702263	0.852944451	1	368	ThermoMPNN
## 108	-7.07594705	0.736358423	1	370	ThermoMPNN
## 109	-10.73643208	1.380139631	1	379	ThermoMPNN
## 110	-14.07207642	1.121161485	1	365	ThermoMPNN
## 111	-9.18200531	1.624652815	1	384	ThermoMPNN
## 112	-11.28864918	0.591423209	1	396	ThermoMPNN
## 113	-12.67210541	0.814016932	1	398	ThermoMPNN

## 114	-9.33935966	1.252710836	1	387	ThermoMPNN
## 115	-13.15141945	0.476879654	0	385	ThermoMPNN
## 116	-12.57753010	0.409772020	0	383	ThermoMPNN
## 117	-12.32525082	0.192949783	0	386	ThermoMPNN
## 118	-10.60443888	0.546977471	0	395	ThermoMPNN
## 119	-12.23365822	0.125742529	0	388	ThermoMPNN
## 120	-15.67217922	0.330956925	0	382	ThermoMPNN
## 121	-14.27076073	1.122033306	1	391	ThermoMPNN
## 122	-8.27435675	1.635041019	1	381	ThermoMPNN
## 123	-10.97792377	0.625834757	1	394	ThermoMPNN
## 124	-10.91672840	1.031781872	1	380	ThermoMPNN
## 125	-8.86661425	1.836252599	1	397	ThermoMPNN
## 126	-10.73927193	0.514175332	0	393	ThermoMPNN
## 127	-7.95011854	0.577652191	1	390	ThermoMPNN
## 128	-12.38695946	-0.012160502	0	399	ThermoMPNN
## 129	-13.43163548	0.288805378	0	392	ThermoMPNN
## 130	-6.53664455	0.862982812	1	409	ThermoMPNN
## 131	-4.56609330	-0.112362143	0	408	ThermoMPNN
## 132	-3.87640061	0.977098956	1	403	ThermoMPNN
## 133	-9.97196865	0.260783789	0	412	ThermoMPNN
## 134	-8.62488279	0.890435095	1	407	ThermoMPNN
## 135	-4.36581016	0.410743668	0	405	ThermoMPNN
## 136	-5.98671331	0.791943611	1	402	ThermoMPNN
## 137	-7.33117771	0.822569952	1	401	ThermoMPNN
## 138	-7.03334475	0.227250171	0	410	ThermoMPNN
## 139	-6.99333563	0.221525601	0	406	ThermoMPNN
## 140	-4.84911342	0.916871330	1	414	ThermoMPNN
## 141	-6.43245831	1.124254357	1	417	ThermoMPNN
## 142	-4.67089536	1.714430382	1	413	ThermoMPNN
## 143	-9.49872723	0.989054506	1	419	ThermoMPNN
## 144	-9.42451019	0.643160767	1	418	ThermoMPNN
## 145	-5.84567728	2.039860442	1	411	ThermoMPNN
## 146	-3.91381145	1.010676758	1	415	ThermoMPNN
## 147	-4.93843803	1.000787840	1	416	ThermoMPNN
## 148	-5.40689783	0.934944709	1	422	ThermoMPNN
## 149	-7.69962387	0.389863804	0	420	ThermoMPNN
## 150	-12.61135521	0.356153397	0	439	ThermoMPNN
## 151	-14.28268890	1.058773018	1	438	ThermoMPNN
## 152	-10.01081676	0.455370519	0	429	ThermoMPNN
## 153	-9.88293228	0.312779246	0	426	ThermoMPNN
## 154	-12.10963936	1.747566748	1	421	ThermoMPNN
## 155	-7.33986340	1.329884724	1	425	ThermoMPNN
## 156	-12.86079426	0.611735943	1	424	ThermoMPNN
## 157	-10.39808445	0.171542347	0	430	ThermoMPNN
## 158	-9.01442490	0.374707751	0	428	ThermoMPNN
## 159	-9.10323019	1.886528232	1	436	ThermoMPNN
## 160	-9.96119556	0.416216937	0	434	ThermoMPNN
## 161	-9.30761547	4.128703297	1	431	ThermoMPNN
## 162	-9.31469650	1.447648941	1	437	ThermoMPNN
## 163	-8.32947435	0.398635754	0	435	ThermoMPNN
## 164	-7.47860956	1.327403066	1	433	ThermoMPNN
## 165	-11.62752953	0.377874651	0	427	ThermoMPNN
## 166	-12.44344387	1.322660600	1	458	ThermoMPNN
## 167	-5.09346228	0.845544008	1	449	ThermoMPNN

## 168	-10.07093344	0.923814922	1	457	ThermoMPNN
## 169	-12.94355297	-0.178397379	0	446	ThermoMPNN
## 170	-14.20928822	0.545153125	0	445	ThermoMPNN
## 171	-9.67660446	1.518308718	1	450	ThermoMPNN
## 172	-14.71240120	0.272402835	0	448	ThermoMPNN
## 173	-14.93833179	-0.135201430	0	451	ThermoMPNN
## 174	-15.06066284	1.501756341	1	442	ThermoMPNN
## 175	-11.95067520	0.226625933	0	455	ThermoMPNN
## 176	-13.08525410	0.645867957	1	456	ThermoMPNN
## 177	-12.91808624	0.214903752	0	440	ThermoMPNN
## 178	-10.51057911	1.060603348	1	441	ThermoMPNN
## 179	-13.48586235	0.205834458	0	454	ThermoMPNN
## 180	-13.55037079	0.558783290	0	453	ThermoMPNN
## 181	-13.91608772	0.083866397	0	452	ThermoMPNN
## 182	-9.30884304	0.985228465	1	464	ThermoMPNN
## 183	-7.42057314	-0.219194340	0	463	ThermoMPNN
## 184	-6.82845697	0.657182328	1	469	ThermoMPNN
## 185	-8.06632938	1.191398044	1	465	ThermoMPNN
## 186	-8.61873331	0.341420566	0	467	ThermoMPNN
## 187	-6.54022322	0.919677267	1	468	ThermoMPNN
## 188	-8.70702524	1.314707795	1	479	ThermoMPNN
## 189	-6.81254730	0.892495477	1	461	ThermoMPNN
## 190	-8.46886072	1.198840293	1	470	ThermoMPNN
## 191	-8.58522940	1.144477400	1	478	ThermoMPNN
## 192	-7.81791668	0.909980050	1	460	ThermoMPNN
## 193	-3.80995698	0.772542974	1	474	ThermoMPNN
## 194	-6.14661083	1.134050254	1	475	ThermoMPNN
## 195	-6.81602621	0.947996141	1	476	ThermoMPNN
## 196	-9.51510944	2.140531414	1	472	ThermoMPNN
## 197	-7.68636312	1.180458341	1	477	ThermoMPNN
## 198	-16.61219063	0.910866124	1	491	ThermoMPNN
## 199	-12.48459854	0.669185322	1	492	ThermoMPNN
## 200	-16.96938782	1.339295999	1	482	ThermoMPNN
## 201	-15.54244366	0.479359406	0	485	ThermoMPNN
## 202	-10.54012928	1.767446124	1	484	ThermoMPNN
## 203	-8.88180122	0.093351355	0	490	ThermoMPNN
## 204	-13.53968182	1.574186166	1	493	ThermoMPNN
## 205	-15.83352146	0.208172548	0	483	ThermoMPNN
## 206	-8.59244699	0.845577619	1	487	ThermoMPNN
## 207	-14.08589230	-0.357268280	0	494	ThermoMPNN
## 208	-14.26332264	0.897759025	1	495	ThermoMPNN
## 209	-12.07900009	0.810422824	1	496	ThermoMPNN
## 210	-13.91746616	0.825749722	1	481	ThermoMPNN
## 211	-14.21951027	0.408768388	0	498	ThermoMPNN
## 212	-14.52641563	0.572220653	1	499	ThermoMPNN
## 213	-14.20505352	0.812954476	1	486	ThermoMPNN
## 214	-7.48033113	0.666022853	1	497	ThermoMPNN
## 215	-15.49502735	0.947278175	1	488	ThermoMPNN
## 216	-12.07907009	0.606760091	1	480	ThermoMPNN
## 217	-5.92686481	0.895045062	1	500	ThermoMPNN
## 218	-6.78738508	1.151816689	1	501	ThermoMPNN
## 219	-7.24847498	1.295766974	1	502	ThermoMPNN
## 220	-10.32045746	1.073399349	1	504	ThermoMPNN
## 221	-8.14886618	1.179794728	1	510	ThermoMPNN

## 222	-6.21088781	2.024359945	1	511	ThermoMPNN
## 223	-4.97627935	0.432585543	0	503	ThermoMPNN
## 224	-3.52674932	1.939302815	1	514	ThermoMPNN
## 225	-3.78369606	2.080534325	1	515	ThermoMPNN
## 226	-4.54546833	0.476010576	0	516	ThermoMPNN
## 227	-6.26989026	1.625611916	1	512	ThermoMPNN
## 228	-3.85077434	0.965253430	1	508	ThermoMPNN
## 229	-6.98397741	1.137818190	1	509	ThermoMPNN
## 230	-5.25200238	1.699677301	1	505	ThermoMPNN
## 231	-9.36375780	1.005748190	1	519	ThermoMPNN
## 232	-8.02664299	0.837102997	1	517	ThermoMPNN
## 233	-10.27795315	1.855813289	1	518	ThermoMPNN
## 234	-9.92690411	0.660521525	1	507	ThermoMPNN
## 235	-7.74720201	-0.015547993	0	528	ThermoMPNN
## 236	-12.06784039	1.045912179	1	524	ThermoMPNN
## 237	-7.80184793	1.160891410	1	535	ThermoMPNN
## 238	-8.58571587	0.839498696	1	529	ThermoMPNN
## 239	-7.78359947	-0.084214020	0	531	ThermoMPNN
## 240	-8.94330692	0.720212346	1	534	ThermoMPNN
## 241	-9.17486696	0.075592314	0	527	ThermoMPNN
## 242	-12.01298695	0.436886151	0	539	ThermoMPNN
## 243	-12.28569813	-0.012862044	0	521	ThermoMPNN
## 244	-7.27591534	1.178795061	1	537	ThermoMPNN
## 245	-7.60042171	1.428625576	1	536	ThermoMPNN
## 246	-12.57360554	0.596523743	1	538	ThermoMPNN
## 247	-6.62785292	0.541250590	0	520	ThermoMPNN
## 248	-6.90614424	2.214869247	1	532	ThermoMPNN
## 249	-8.43976946	1.786298300	1	530	ThermoMPNN
## 250	-6.54060898	0.884022535	1	525	ThermoMPNN
## 251	-7.15670729	0.928950656	1	533	ThermoMPNN
## 252	-9.23508825	0.997862722	1	526	ThermoMPNN
## 253	-6.46101370	0.771375399	1	553	ThermoMPNN
## 254	-9.41816492	1.469016695	1	552	ThermoMPNN
## 255	-8.68342314	0.705238350	1	557	ThermoMPNN
## 256	-7.18413258	1.329208492	1	540	ThermoMPNN
## 257	-8.89015665	0.935917409	1	551	ThermoMPNN
## 258	-8.09011097	0.769510222	1	548	ThermoMPNN
## 259	-11.32040987	1.295410891	1	547	ThermoMPNN
## 260	-8.36652651	0.911904105	1	555	ThermoMPNN
## 261	-12.41282711	0.177049335	0	558	ThermoMPNN
## 262	-10.53723373	1.696038987	1	550	ThermoMPNN
## 263	-9.12860451	1.666772337	1	556	ThermoMPNN
## 264	-8.88058996	2.266190939	1	546	ThermoMPNN
## 265	-6.99881458	1.359430782	1	545	ThermoMPNN
## 266	-11.03663874	0.636728571	1	541	ThermoMPNN
## 267	-9.78825169	0.944435463	1	549	ThermoMPNN
## 268	-12.29379215	0.781461371	1	544	ThermoMPNN
## 269	-5.57315912	0.747265022	1	542	ThermoMPNN
## 270	-8.73592739	0.795568082	1	554	ThermoMPNN
## 271	-11.67783384	0.698599201	1	559	ThermoMPNN
## 272	-7.75493956	1.201157473	1	575	ThermoMPNN
## 273	-6.46771431	-0.375193540	0	573	ThermoMPNN
## 274	-10.44271450	1.587574916	1	561	ThermoMPNN
## 275	-8.28256063	1.158877089	1	574	ThermoMPNN

## 276	-9.11875534	1.982881097	1	569	ThermoMPNN
## 277	-7.70915480	1.204591318	1	577	ThermoMPNN
## 278	-7.47048321	0.849224802	1	576	ThermoMPNN
## 279	-5.53259244	1.124955546	1	563	ThermoMPNN
## 280	-6.74433732	0.758295479	1	568	ThermoMPNN
## 281	-9.74055901	0.311636118	0	567	ThermoMPNN
## 282	-7.18665867	0.964248481	1	560	ThermoMPNN
## 283	-10.44373741	0.606917060	1	572	ThermoMPNN
## 284	-9.17119207	0.203727712	0	570	ThermoMPNN
## 285	-11.12014961	1.470250135	1	564	ThermoMPNN
## 286	-12.54341431	1.461090001	1	578	ThermoMPNN
## 287	-7.32136140	0.498957145	0	565	ThermoMPNN
## 288	-12.90125542	0.705471089	1	594	ThermoMPNN
## 289	-13.26045036	0.550057565	0	593	ThermoMPNN
## 290	-13.66995602	0.557235513	0	581	ThermoMPNN
## 291	-14.27412224	0.722486170	1	592	ThermoMPNN
## 292	-13.37794037	0.045302997	0	580	ThermoMPNN
## 293	-16.27090683	1.516342193	1	585	ThermoMPNN
## 294	-14.06417942	1.556260436	1	595	ThermoMPNN
## 295	-16.59443092	0.968119194	1	591	ThermoMPNN
## 296	-14.52918358	1.119971233	1	599	ThermoMPNN
## 297	-16.99363708	1.106491379	1	583	ThermoMPNN
## 298	-12.93155136	1.634661926	1	596	ThermoMPNN
## 299	-19.00390930	1.151407716	1	582	ThermoMPNN
## 300	-10.36465034	1.426571732	1	584	ThermoMPNN
## 301	-14.24658432	0.753137206	1	588	ThermoMPNN
## 302	-13.72095013	0.768971027	1	598	ThermoMPNN
## 303	-14.42620354	0.725965790	1	586	ThermoMPNN
## 304	-8.72807121	0.559150334	0	597	ThermoMPNN
## 305	-8.91982498	0.517143623	0	587	ThermoMPNN
## 306	-11.75329590	1.067341603	1	619	ThermoMPNN
## 307	-8.87274599	1.213464538	1	618	ThermoMPNN
## 308	-8.57847433	1.406676547	1	616	ThermoMPNN
## 309	-9.73703318	0.948020181	1	600	ThermoMPNN
## 310	-9.99899349	0.931074261	1	617	ThermoMPNN
## 311	-9.03772907	1.065376617	1	615	ThermoMPNN
## 312	-11.12130127	-0.103747095	0	602	ThermoMPNN
## 313	-8.32862492	0.649868595	1	611	ThermoMPNN
## 314	-12.62402725	0.491587468	0	604	ThermoMPNN
## 315	-10.33552170	0.847247645	1	601	ThermoMPNN
## 316	-12.47987347	0.294216906	0	612	ThermoMPNN
## 317	-10.12353153	0.793578151	1	607	ThermoMPNN
## 318	-8.50331831	1.181665171	1	603	ThermoMPNN
## 319	-4.63244352	1.070186800	1	614	ThermoMPNN
## 320	-6.55915775	0.630421742	1	613	ThermoMPNN
## 321	-8.99563007	1.601256248	1	609	ThermoMPNN
## 322	-9.24898882	0.367625103	0	605	ThermoMPNN
## 323	-8.78871679	1.229406487	1	606	ThermoMPNN
## 324	-7.14693680	1.094894940	1	635	ThermoMPNN
## 325	-4.85458121	1.213163755	1	634	ThermoMPNN
## 326	-7.01080065	1.464539667	1	636	ThermoMPNN
## 327	-7.04722414	0.899722654	1	625	ThermoMPNN
## 328	-6.94330039	1.508554586	1	620	ThermoMPNN
## 329	-9.34712887	1.238634717	1	621	ThermoMPNN

## 330	-7.96852436	0.892987276	1	637	ThermoMPNN
## 331	-6.89792089	1.649543449	1	622	ThermoMPNN
## 332	-7.39646740	0.355062635	0	626	ThermoMPNN
## 333	-8.61689119	-0.005519382	0	627	ThermoMPNN
## 334	-10.49654999	0.292105337	0	639	ThermoMPNN
## 335	-5.10258636	1.115715011	1	633	ThermoMPNN
## 336	-5.20595751	1.426452919	1	623	ThermoMPNN
## 337	-10.82412262	0.963609265	1	624	ThermoMPNN
## 338	-9.58483267	0.354850749	0	638	ThermoMPNN
## 339	-6.94900265	0.916136220	1	629	ThermoMPNN
## 340	-7.11378570	0.929918690	1	630	ThermoMPNN
## 341	-10.64496756	0.072117544	0	632	ThermoMPNN
## 342	-9.58917274	0.546897506	0	640	ThermoMPNN
## 343	-13.23189621	0.452663684	0	641	ThermoMPNN
## 344	-14.27539864	-0.213700031	0	643	ThermoMPNN
## 345	-12.02993126	0.343381641	0	644	ThermoMPNN
## 346	-13.99061718	1.178022841	1	645	ThermoMPNN
## 347	-15.76357193	-0.370485710	0	646	ThermoMPNN
## 348	-5.56162071	0.538669405	0	647	ThermoMPNN
## 349	-15.21200466	-0.100709373	0	648	ThermoMPNN
## 350	-9.11699429	0.966150613	1	649	ThermoMPNN
## 351	-9.07996941	0.740303899	1	650	ThermoMPNN
## 352	-14.27649193	0.157544637	0	651	ThermoMPNN
## 353	-15.42872734	0.134454104	0	652	ThermoMPNN
## 354	-15.41557350	0.756933591	1	653	ThermoMPNN
## 355	-14.95233803	0.009032334	0	654	ThermoMPNN
## 356	-13.10905380	0.505059519	0	655	ThermoMPNN
## 357	-10.17667007	0.700549498	1	656	ThermoMPNN
## 358	-16.38422699	-0.340559151	0	658	ThermoMPNN
## 359	-14.84251881	-0.145974982	0	659	ThermoMPNN
## 360	-16.10637779	0.086630190	0	672	ThermoMPNN
## 361	-13.37936020	1.049529871	1	671	ThermoMPNN
## 362	-14.63089771	1.319375341	1	663	ThermoMPNN
## 363	-14.66084251	0.044764634	0	666	ThermoMPNN
## 364	-9.35884933	1.396154170	1	669	ThermoMPNN
## 365	-13.75258083	0.745791539	1	661	ThermoMPNN
## 366	-13.75201588	0.564872199	1	665	ThermoMPNN
## 367	-12.47046566	0.813780458	1	673	ThermoMPNN
## 368	-15.09888306	0.359394239	0	679	ThermoMPNN
## 369	-10.87900734	0.858415476	1	675	ThermoMPNN
## 370	-7.84867773	0.753527929	1	677	ThermoMPNN
## 371	-14.16648121	1.723387206	1	678	ThermoMPNN
## 372	-10.01212311	0.474391875	0	660	ThermoMPNN
## 373	-7.47995481	0.294086146	0	676	ThermoMPNN
## 374	-12.21963196	0.745186634	1	674	ThermoMPNN
## 375	-16.56812496	1.072501290	1	662	ThermoMPNN
## 376	-5.94123783	0.659682472	1	685	ThermoMPNN
## 377	-9.48543320	1.364131260	1	701	ThermoMPNN
## 378	-10.18181915	1.086956156	1	700	ThermoMPNN
## 379	-9.54404593	0.925750126	1	715	ThermoMPNN
## 380	-10.57789650	0.703936139	1	716	ThermoMPNN
## 381	-14.68362713	-0.331324454	0	712	ThermoMPNN
## 382	-8.54154854	0.831972326	1	713	ThermoMPNN
## 383	-10.55317421	0.083524420	0	705	ThermoMPNN

## 384	-7.71774063	0.532758471	0	706	ThermoMPNN
## 385	-11.29994831	1.030646024	1	703	ThermoMPNN
## 386	-12.96508884	0.422960669	0	704	ThermoMPNN
## 387	-10.20379047	1.152305649	1	709	ThermoMPNN
## 388	-10.95353184	0.199848432	0	710	ThermoMPNN
## 389	-10.49113884	0.170249753	0	711	ThermoMPNN
## 390	-11.61706066	0.761599740	1	707	ThermoMPNN
## 391	-8.52819872	1.664320145	1	708	ThermoMPNN
## 392	-11.46576996	0.571017238	1	717	ThermoMPNN
## 393	-11.79766235	1.068660231	1	719	ThermoMPNN
## 394	-13.51329117	0.685481475	1	739	ThermoMPNN
## 395	-17.83031578	-0.739356292	0	722	ThermoMPNN
## 396	-9.20826626	0.261672740	0	737	ThermoMPNN
## 397	-14.26959858	-0.238955815	0	738	ThermoMPNN
## 398	-16.83896179	-0.256500755	0	723	ThermoMPNN
## 399	-5.93770790	0.270462970	0	724	ThermoMPNN
## 400	-13.65442657	-0.255559273	0	720	ThermoMPNN
## 401	-14.42933025	0.674145277	1	721	ThermoMPNN
## 402	-14.20810165	-0.243937068	0	735	ThermoMPNN
## 403	-11.75555916	0.693255040	1	736	ThermoMPNN
## 404	-8.24896412	0.742177925	1	727	ThermoMPNN
## 405	-15.20929642	-0.444173792	0	734	ThermoMPNN
## 406	-15.15729275	-0.332987669	0	733	ThermoMPNN
## 407	-15.95188198	-0.087235902	0	726	ThermoMPNN
## 408	-5.86018381	0.882608856	1	729	ThermoMPNN
## 409	-16.75108204	-0.137904582	0	725	ThermoMPNN
## 410	-15.94172440	0.272313736	0	731	ThermoMPNN
## 411	-15.67819080	0.049282285	0	732	ThermoMPNN
## 412	-11.88691463	1.089394636	1	741	ThermoMPNN
## 413	-11.17728310	0.678182451	1	745	ThermoMPNN
## 414	-11.89303436	0.645395985	1	742	ThermoMPNN
## 415	-9.50600128	1.272028024	1	743	ThermoMPNN
## 416	-9.67573395	1.128707678	1	740	ThermoMPNN
## 417	-10.18785610	1.044327156	1	755	ThermoMPNN
## 418	-9.09779530	0.903228828	1	756	ThermoMPNN
## 419	-13.34566536	0.397811208	0	744	ThermoMPNN
## 420	-12.06958370	1.162096182	1	758	ThermoMPNN
## 421	-11.82987137	0.561129072	0	759	ThermoMPNN
## 422	-8.18317432	0.583057173	1	746	ThermoMPNN
## 423	-9.19505577	0.891587077	1	757	ThermoMPNN
## 424	-14.42556229	0.129542209	0	752	ThermoMPNN
## 425	-7.65474319	0.760941696	1	754	ThermoMPNN
## 426	-9.02809114	1.086682892	1	749	ThermoMPNN
## 427	-9.41074409	0.367024039	0	750	ThermoMPNN
## 428	-9.92642384	0.651089773	1	747	ThermoMPNN
## 429	-8.53938904	0.354029683	0	748	ThermoMPNN
## 430	-10.78791256	0.815865197	1	751	ThermoMPNN
## 431	-7.75772886	1.215379613	1	777	ThermoMPNN
## 432	-10.61915150	1.284594321	1	778	ThermoMPNN
## 433	-11.17303810	0.782400537	1	764	ThermoMPNN
## 434	-6.94857817	0.630763384	1	776	ThermoMPNN
## 435	-8.13056879	1.018470057	1	766	ThermoMPNN
## 436	-6.59327540	1.132668424	1	763	ThermoMPNN
## 437	-7.56790113	1.201922199	1	765	ThermoMPNN

## 438	-8.19853020	0.366359969	0	762	ThermoMPNN
## 439	-7.64756508	1.138442603	1	770	ThermoMPNN
## 440	-7.47960148	1.586409208	1	771	ThermoMPNN
## 441	-10.87389164	0.197770802	0	779	ThermoMPNN
## 442	-10.38284111	0.844136077	1	761	ThermoMPNN
## 443	-9.13980675	1.345270914	1	767	ThermoMPNN
## 444	-7.93466749	0.888145353	1	769	ThermoMPNN
## 445	-7.13698473	0.555761726	0	775	ThermoMPNN
## 446	-13.87718811	0.304323777	0	772	ThermoMPNN
## 447	-5.32202454	1.456011641	1	774	ThermoMPNN
## 448	-6.50693674	1.514973726	1	760	ThermoMPNN
## 449	-5.85777025	0.908788580	1	773	ThermoMPNN
## 450	-12.87804832	0.204946336	0	788	ThermoMPNN
## 451	-15.12366066	-0.265743438	0	786	ThermoMPNN
## 452	-12.55526848	2.417941729	1	785	ThermoMPNN
## 453	-16.95103397	-0.035941424	0	784	ThermoMPNN
## 454	-14.37117310	0.544859252	0	790	ThermoMPNN
## 455	-14.63481178	0.854826459	1	787	ThermoMPNN
## 456	-13.59459057	0.655312635	1	791	ThermoMPNN
## 457	-14.88664207	0.062618959	0	789	ThermoMPNN
## 458	-19.34602051	-0.071607486	0	792	ThermoMPNN
## 459	-11.06395721	1.441831463	1	780	ThermoMPNN
## 460	-8.49331722	1.277994064	1	782	ThermoMPNN
## 461	-15.76855373	0.164245249	0	794	ThermoMPNN
## 462	-16.34953556	1.178584160	1	781	ThermoMPNN
## 463	-14.18301010	0.871315280	1	795	ThermoMPNN
## 464	-16.18307209	-0.076335715	0	799	ThermoMPNN
## 465	-17.53467979	-0.080158397	0	798	ThermoMPNN
## 466	-13.53589268	0.593322395	1	796	ThermoMPNN
## 467	-11.43840771	0.128228834	0	797	ThermoMPNN
## 468	-19.15989838	-0.263608565	0	802	ThermoMPNN
## 469	-16.61302853	0.716708691	1	801	ThermoMPNN
## 470	-17.58969688	0.363696120	0	803	ThermoMPNN
## 471	-18.24827843	-0.000404364	0	805	ThermoMPNN
## 472	-11.92354565	1.140259811	1	816	ThermoMPNN
## 473	-12.53950958	0.898328745	1	804	ThermoMPNN
## 474	-14.72090664	0.523141508	0	800	ThermoMPNN
## 475	-15.37023067	-0.168826558	0	814	ThermoMPNN
## 476	-15.58054409	0.252821758	0	815	ThermoMPNN
## 477	-10.39747810	0.284522282	0	817	ThermoMPNN
## 478	-16.59331627	-0.075254656	0	818	ThermoMPNN
## 479	-15.49862804	0.828102148	1	813	ThermoMPNN
## 480	-16.58795414	0.085202424	0	819	ThermoMPNN
## 481	-17.62658386	-0.036966430	0	806	ThermoMPNN
## 482	-7.86610584	0.967126360	1	809	ThermoMPNN
## 483	-16.91439362	0.071085537	0	812	ThermoMPNN
## 484	-8.59918795	0.860003410	1	837	ThermoMPNN
## 485	-8.38857937	1.288930685	1	835	ThermoMPNN
## 486	-15.78548889	0.228891512	0	832	ThermoMPNN
## 487	-10.54879818	1.075374078	1	830	ThermoMPNN
## 488	-9.48159065	0.581264768	1	833	ThermoMPNN
## 489	-13.79720440	1.304671508	1	838	ThermoMPNN
## 490	-11.40096054	0.787373775	1	839	ThermoMPNN
## 491	-9.55289879	1.794364323	1	828	ThermoMPNN

## 492	-10.68025589	0.953645179	1	829	ThermoMPNN
## 493	-10.50529652	1.184842343	1	834	ThermoMPNN
## 494	-6.89628468	1.293218461	1	831	ThermoMPNN
## 495	-12.17218876	0.775298787	1	821	ThermoMPNN
## 496	-10.17243853	1.049154847	1	827	ThermoMPNN
## 497	-6.87182665	1.067487945	1	820	ThermoMPNN
## 498	-8.45516357	1.163797489	1	825	ThermoMPNN
## 499	-12.39007273	1.250094081	1	824	ThermoMPNN
## 500	-8.17007875	2.684322880	1	836	ThermoMPNN
## 501	-5.45448265	0.697100727	1	823	ThermoMPNN
## 502	-8.21090059	0.590381852	1	840	ThermoMPNN
## 503	-14.09883785	-0.061872294	0	852	ThermoMPNN
## 504	-8.80342197	0.442897220	0	849	ThermoMPNN
## 505	-8.74591446	0.870476129	1	850	ThermoMPNN
## 506	-9.35187111	0.749931206	1	851	ThermoMPNN
## 507	-9.62660065	1.444985834	1	843	ThermoMPNN
## 508	-9.07695913	0.804227198	1	855	ThermoMPNN
## 509	-10.23116226	1.139248802	1	841	ThermoMPNN
## 510	-11.06168289	0.114745459	0	842	ThermoMPNN
## 511	-9.71476059	0.651412744	1	847	ThermoMPNN
## 512	-4.75201120	0.251356329	0	848	ThermoMPNN
## 513	-12.59058571	1.277593637	1	844	ThermoMPNN
## 514	-10.53255196	0.228226165	0	845	ThermoMPNN
## 515	-8.86645775	1.407992533	1	856	ThermoMPNN
## 516	-9.17521563	1.384636112	1	857	ThermoMPNN
## 517	-9.21544075	0.560145158	0	846	ThermoMPNN
## 518	-12.37571907	1.441686632	1	859	ThermoMPNN
## 519	-11.44374695	0.816778477	1	858	ThermoMPNN
## 520	-16.15827942	-0.194888095	0	868	ThermoMPNN
## 521	-17.03410072	0.035857075	0	867	ThermoMPNN
## 522	-17.18278675	0.354445406	0	866	ThermoMPNN
## 523	-17.85492229	-0.378224986	0	864	ThermoMPNN
## 524	-13.44167824	0.442993183	0	860	ThermoMPNN
## 525	-17.12512703	-0.128884884	0	870	ThermoMPNN
## 526	-18.35141392	-0.110518259	0	879	ThermoMPNN
## 527	-15.30192509	0.766944507	1	878	ThermoMPNN
## 528	-14.86206532	0.011596350	0	877	ThermoMPNN
## 529	-14.31957874	-0.372799293	0	863	ThermoMPNN
## 530	-16.30502987	0.170023449	0	869	ThermoMPNN
## 531	-16.16618061	-0.168056330	0	876	ThermoMPNN
## 532	-12.99160614	-0.379372919	0	875	ThermoMPNN
## 533	-19.44777145	-0.667325056	0	872	ThermoMPNN
## 534	-12.96299019	0.074637637	0	874	ThermoMPNN
## 535	-15.47174625	0.665116044	1	871	ThermoMPNN
## 536	-17.13579369	0.399580229	0	873	ThermoMPNN
## 537	-15.76490288	0.883259289	1	895	ThermoMPNN
## 538	-15.50343113	-0.092570980	0	896	ThermoMPNN
## 539	-16.66276608	0.548545613	0	880	ThermoMPNN
## 540	-15.12876892	0.151943064	0	894	ThermoMPNN
## 541	-18.65184822	-0.043462938	0	882	ThermoMPNN
## 542	-15.69923668	-0.003961914	0	898	ThermoMPNN
## 543	-16.48838253	0.251707029	0	881	ThermoMPNN
## 544	-11.86608486	-0.142872617	0	887	ThermoMPNN
## 545	-12.88100719	0.025174008	0	897	ThermoMPNN

## 546	-15.11860199	-0.286777200	0	893	ThermoMPNN
## 547	-16.20481014	-0.035105666	0	886	ThermoMPNN
## 548	-17.38813477	-0.195028744	0	885	ThermoMPNN
## 549	-17.57225876	-0.211950800	0	883	ThermoMPNN
## 550	-14.81028385	0.279883423	0	892	ThermoMPNN
## 551	-16.87232208	0.080659325	0	888	ThermoMPNN
## 552	-16.91423111	-0.211099291	0	899	ThermoMPNN
## 553	-18.03451118	-0.008837313	0	891	ThermoMPNN
## 554	-9.22792530	0.926977104	1	903	ThermoMPNN
## 555	-7.11639075	1.423323003	1	900	ThermoMPNN
## 556	-8.27743893	0.562875681	0	901	ThermoMPNN
## 557	-10.86588402	1.241451846	1	902	ThermoMPNN
## 558	-8.77051868	1.562231486	1	916	ThermoMPNN
## 559	-11.70580845	-0.440743731	0	912	ThermoMPNN
## 560	-6.38709011	0.218584764	0	913	ThermoMPNN
## 561	-6.32046099	1.402937365	1	915	ThermoMPNN
## 562	-7.12031736	1.494599625	1	906	ThermoMPNN
## 563	-10.13720646	0.385534794	0	917	ThermoMPNN
## 564	-11.35044651	0.932735024	1	904	ThermoMPNN
## 565	-7.57077003	1.369918658	1	905	ThermoMPNN
## 566	-9.61796179	0.754672993	1	910	ThermoMPNN
## 567	-8.55939627	1.203908907	1	911	ThermoMPNN
## 568	-11.01264858	0.747465943	1	907	ThermoMPNN
## 569	-5.10956974	0.698844425	1	908	ThermoMPNN
## 570	-10.61708355	0.210382397	0	918	ThermoMPNN
## 571	-11.03333969	0.452005369	0	919	ThermoMPNN
## 572	-8.49449568	0.512533353	0	909	ThermoMPNN
## 573	-9.30002661	0.567383488	1	926	ThermoMPNN
## 574	-11.25612745	0.867899534	1	925	ThermoMPNN
## 575	-11.67010365	1.188324189	1	939	ThermoMPNN
## 576	-11.32707901	0.964334560	1	938	ThermoMPNN
## 577	-5.38170080	1.494257197	1	928	ThermoMPNN
## 578	-7.69900303	0.754023269	1	927	ThermoMPNN
## 579	-12.24835348	0.070704240	0	922	ThermoMPNN
## 580	-10.16507730	0.352227468	0	923	ThermoMPNN
## 581	-10.26224651	1.187315279	1	924	ThermoMPNN
## 582	-6.52787867	0.801248246	1	937	ThermoMPNN
## 583	-9.09488621	1.161740852	1	936	ThermoMPNN
## 584	-7.86312904	0.692142300	1	933	ThermoMPNN
## 585	-10.39195948	0.405958889	0	932	ThermoMPNN
## 586	-5.79147832	1.609096384	1	934	ThermoMPNN
## 587	-6.57092133	1.183187824	1	930	ThermoMPNN
## 588	-9.36433849	1.547152317	1	920	ThermoMPNN
## 589	-9.78090706	1.218493689	1	935	ThermoMPNN
## 590	-10.28694334	0.692328738	1	931	ThermoMPNN
## 591	-11.10329809	1.609222293	1	921	ThermoMPNN
## 592	-9.32143736	1.409635470	1	951	ThermoMPNN
## 593	-9.57357674	0.322787322	0	955	ThermoMPNN
## 594	-6.50640445	0.295165138	0	942	ThermoMPNN
## 595	-10.22028885	0.517644647	0	949	ThermoMPNN
## 596	-10.56286526	0.770019107	1	952	ThermoMPNN
## 597	-9.03744764	0.570058678	1	945	ThermoMPNN
## 598	-9.54207115	0.553957407	0	946	ThermoMPNN
## 599	-11.66095619	1.618242355	1	947	ThermoMPNN

## 600	-10.25234060	1.213138485	1	954	ThermoMPNN
## 601	-10.01471262	1.356895365	1	956	ThermoMPNN
## 602	-9.61113577	0.832335046	1	957	ThermoMPNN
## 603	-9.14535007	1.065902549	1	940	ThermoMPNN
## 604	-10.05032883	0.447104018	0	960	ThermoMPNN
## 605	-13.39852734	0.397618520	0	961	ThermoMPNN
## 606	-13.91761684	1.128305254	1	962	ThermoMPNN
## 607	-14.79627571	0.095108005	0	963	ThermoMPNN
## 608	-15.29488182	0.817751250	1	964	ThermoMPNN
## 609	-13.20487080	1.581450450	1	965	ThermoMPNN
## 610	-14.45270081	0.075145562	0	966	ThermoMPNN
## 611	-11.72979164	0.613184331	1	967	ThermoMPNN
## 612	-13.00236645	1.202816978	1	968	ThermoMPNN
## 613	-13.46400604	1.037340874	1	969	ThermoMPNN
## 614	-11.94816132	0.484534538	0	970	ThermoMPNN
## 615	-11.05111294	0.366487999	0	971	ThermoMPNN
## 616	-13.50586452	0.038777586	0	972	ThermoMPNN
## 617	-14.84578953	0.206662110	0	973	ThermoMPNN
## 618	-12.48278942	1.169002066	1	974	ThermoMPNN
## 619	-8.08868198	1.136888018	1	975	ThermoMPNN
## 620	-13.30904121	0.596848083	1	977	ThermoMPNN
## 621	-16.69853649	0.808017202	1	978	ThermoMPNN
## 622	-11.33246193	0.232143714	0	982	ThermoMPNN
## 623	-12.80064983	0.112529936	0	980	ThermoMPNN
## 624	-12.63396358	-0.077207071	0	983	ThermoMPNN
## 625	-10.70387001	0.021195265	0	981	ThermoMPNN
## 626	-13.79295979	0.055352742	0	997	ThermoMPNN
## 627	-9.49360580	0.136754066	0	994	ThermoMPNN
## 628	-14.25153408	-0.151810918	0	998	ThermoMPNN
## 629	-12.41174202	0.332009293	0	984	ThermoMPNN
## 630	-14.31539021	-0.006510269	0	987	ThermoMPNN
## 631	-13.00528107	0.376862881	0	996	ThermoMPNN
## 632	-8.41469336	1.476961943	1	993	ThermoMPNN
## 633	-11.47333832	0.323644701	0	985	ThermoMPNN
## 634	-9.55114861	0.177273624	0	999	ThermoMPNN
## 635	-14.34098186	0.247867398	0	990	ThermoMPNN
## 636	-11.97937546	-0.008267905	0	988	ThermoMPNN
## 637	-10.80056572	0.275913989	0	995	ThermoMPNN
## 638	-12.43161335	-0.018966311	0	992	ThermoMPNN
## 639	-11.83844891	0.065607585	0	989	ThermoMPNN
## 640	-10.48187675	0.345356108	0	1010	ThermoMPNN
## 641	-7.31915445	0.259679297	0	1008	ThermoMPNN
## 642	-9.27089081	0.917902821	1	1014	ThermoMPNN
## 643	-9.78600178	2.234338941	1	1006	ThermoMPNN
## 644	-10.50630960	0.726476307	1	1009	ThermoMPNN
## 645	-13.53936901	0.884043909	1	1018	ThermoMPNN
## 646	-11.79518509	0.749385908	1	1007	ThermoMPNN
## 647	-9.69881430	1.492864448	1	1015	ThermoMPNN
## 648	-10.28639927	0.719048766	1	1016	ThermoMPNN
## 649	-9.90304346	0.676822124	1	1017	ThermoMPNN
## 650	-8.54128714	1.088351197	1	1000	ThermoMPNN
## 651	-9.52981253	1.350311357	1	1005	ThermoMPNN
## 652	-9.50621729	0.410256666	0	1011	ThermoMPNN
## 653	-8.55689392	0.826897073	1	1012	ThermoMPNN

## 654	-7.48046303	1.169228857	1 1013	ThermoMPNN
## 655	-13.59476357	0.519876388	0 1004	ThermoMPNN
## 656	-12.54629536	0.801950281	1 1019	ThermoMPNN
## 657	-13.07767792	1.191724712	1 1001	ThermoMPNN
## 658	-9.77193594	0.914231992	1 1034	ThermoMPNN
## 659	-7.09437895	0.952491555	1 1028	ThermoMPNN
## 660	-13.30625172	0.900615111	1 1039	ThermoMPNN
## 661	-11.47345276	0.877311665	1 1029	ThermoMPNN
## 662	-8.04609566	0.555412965	0 1033	ThermoMPNN
## 663	-9.23051119	0.839471614	1 1036	ThermoMPNN
## 664	-14.73741016	0.705172377	1 1038	ThermoMPNN
## 665	-9.03817444	2.241514662	1 1030	ThermoMPNN
## 666	-11.62122240	1.194995501	1 1027	ThermoMPNN
## 667	-10.11673107	0.913634862	1 1035	ThermoMPNN
## 668	-12.17750340	0.976981564	1 1032	ThermoMPNN
## 669	-13.45990067	0.788438245	1 1021	ThermoMPNN
## 670	-10.56890497	1.466334122	1 1026	ThermoMPNN
## 671	-9.09297104	0.607741800	1 1025	ThermoMPNN
## 672	-9.55654583	0.622908848	1 1020	ThermoMPNN
## 673	-7.60612516	0.923221130	1 1022	ThermoMPNN
## 674	-14.56479473	0.879753028	1 1024	ThermoMPNN
## 675	-10.45248394	0.863192153	1 1037	ThermoMPNN
## 676	-14.48355980	0.117807592	0 1046	ThermoMPNN
## 677	-14.62288895	-0.406761268	0 1050	ThermoMPNN
## 678	-14.52541218	-0.003672805	0 1049	ThermoMPNN
## 679	-10.05425053	0.290864082	0 1056	ThermoMPNN
## 680	-16.47411232	-0.090607393	0 1058	ThermoMPNN
## 681	-11.41311893	0.114296467	0 1057	ThermoMPNN
## 682	-14.65380344	0.275709838	0 1053	ThermoMPNN
## 683	-10.08516436	-0.151869110	0 1045	ThermoMPNN
## 684	-13.80457897	-0.209881332	0 1051	ThermoMPNN
## 685	-12.08750896	0.086347547	0 1052	ThermoMPNN
## 686	-15.06622887	0.624691241	1 1048	ThermoMPNN
## 687	-14.57454453	0.063894904	0 1047	ThermoMPNN
## 688	-8.48952494	0.381688116	0 1055	ThermoMPNN
## 689	-12.70378799	0.621089100	1 1041	ThermoMPNN
## 690	-13.01724720	0.170535513	0 1043	ThermoMPNN
## 691	-14.99853477	0.262989409	0 1044	ThermoMPNN
## 692	-15.09864960	0.420593520	0 1059	ThermoMPNN
## 693	-14.23515167	0.224854051	0 1054	ThermoMPNN
## 694	-7.51783628	0.561295856	0 1060	ThermoMPNN
## 695	-8.42796078	0.819063611	1 1061	ThermoMPNN
## 696	-11.74746227	0.666443335	1 1062	ThermoMPNN
## 697	-12.73623543	0.603731457	1 1063	ThermoMPNN
## 698	-10.88264656	0.421331899	0 1064	ThermoMPNN
## 699	-9.10672560	0.574826018	1 1065	ThermoMPNN
## 700	-11.93642063	1.268879762	1 1066	ThermoMPNN
## 701	-11.29400501	0.863795290	1 1067	ThermoMPNN
## 702	-12.17842579	0.182387307	0 1068	ThermoMPNN
## 703	-10.75986443	0.145765645	0 1069	ThermoMPNN
## 704	-12.38111744	0.840342877	1 1070	ThermoMPNN
## 705	-9.78907490	0.595493777	1 1072	ThermoMPNN
## 706	-12.25681763	1.440934918	1 1073	ThermoMPNN
## 707	-11.41105480	0.747152568	1 1074	ThermoMPNN

## 708	-8.99547501	2.433943617	1 1076	ThermoMPNN
## 709	-10.81824455	1.135540743	1 1077	ThermoMPNN
## 710	-13.74122696	0.363748672	0 1078	ThermoMPNN
## 711	-12.08752689	0.287922451	0 1079	ThermoMPNN
## 712	-11.46304226	0.005048935	0 1080	ThermoMPNN
## 713	-14.60245171	0.703222519	1 1081	ThermoMPNN
## 714	-14.70731125	-0.150617288	0 1083	ThermoMPNN
## 715	-14.61354065	-0.039406021	0 1085	ThermoMPNN
## 716	-16.12987652	-0.312774160	0 1086	ThermoMPNN
## 717	-15.21002274	0.011918427	0 1088	ThermoMPNN
## 718	-8.66667681	0.642665478	1 1089	ThermoMPNN
## 719	-10.10160637	0.223497345	0 1090	ThermoMPNN
## 720	-15.37468739	0.306109150	0 1091	ThermoMPNN
## 721	-14.89980049	0.012110573	0 1092	ThermoMPNN
## 722	-14.95276909	-0.080424752	0 1093	ThermoMPNN
## 723	-14.98990574	0.233822254	0 1094	ThermoMPNN
## 724	-14.92281418	0.055944975	0 1095	ThermoMPNN
## 725	-12.38848629	0.376056931	0 1096	ThermoMPNN
## 726	-16.54984550	0.277803770	0 1098	ThermoMPNN
## 727	-15.78988609	0.043237502	0 1099	ThermoMPNN
## 728	-9.67454386	0.174901996	0 1114	ThermoMPNN
## 729	-14.13402538	0.564359094	1 1115	ThermoMPNN
## 730	-11.20074348	1.671068228	1 1113	ThermoMPNN
## 731	-15.23069305	0.858675047	1 1105	ThermoMPNN
## 732	-15.64898796	0.375848254	0 1101	ThermoMPNN
## 733	-12.92893906	0.383015077	0 1103	ThermoMPNN
## 734	-18.18369064	0.413938856	0 1104	ThermoMPNN
## 735	-14.89746723	0.960012901	1 1100	ThermoMPNN
## 736	-15.21129513	0.767517825	1 1112	ThermoMPNN
## 737	-14.66882286	0.413286172	0 1106	ThermoMPNN
## 738	-16.09311752	0.183172813	0 1102	ThermoMPNN
## 739	-12.84493656	-0.012679819	0 1116	ThermoMPNN
## 740	-15.97258606	0.009555660	0 1117	ThermoMPNN
## 741	-16.34831581	-0.026027833	0 1118	ThermoMPNN
## 742	-14.62214603	0.172325241	0 1107	ThermoMPNN
## 743	-15.01151047	0.342420396	0 1109	ThermoMPNN
## 744	-17.66335011	0.050509730	0 1119	ThermoMPNN
## 745	-15.95711975	-0.059960497	0 1126	ThermoMPNN
## 746	-12.69771366	-0.081699748	0 1127	ThermoMPNN
## 747	-16.41511784	-0.041916445	0 1125	ThermoMPNN
## 748	-15.08452568	-0.157193781	0 1138	ThermoMPNN
## 749	-13.79543934	-0.229449939	0 1124	ThermoMPNN
## 750	-16.27108593	0.161106131	0 1131	ThermoMPNN
## 751	-15.79167423	0.118544527	0 1132	ThermoMPNN
## 752	-12.14710541	0.091503291	0 1129	ThermoMPNN
## 753	-16.32809124	1.220675871	1 1123	ThermoMPNN
## 754	-15.01566010	0.155925356	0 1120	ThermoMPNN
## 755	-10.40229931	1.530128429	1 1121	ThermoMPNN
## 756	-16.33101902	-0.162352046	0 1139	ThermoMPNN
## 757	-18.45100861	0.233575584	0 1122	ThermoMPNN
## 758	-14.11781731	0.444087214	0 1136	ThermoMPNN
## 759	-14.05252876	-0.063963686	0 1137	ThermoMPNN
## 760	-14.08312454	-0.065848866	0 1134	ThermoMPNN
## 761	-14.07532234	0.379122215	0 1135	ThermoMPNN

## 762	-13.19510059	0.088572615	0 1133	ThermoMPNN
## 763	-15.38197384	-0.126657318	0 1140	ThermoMPNN
## 764	-13.64483643	-0.061516289	0 1141	ThermoMPNN
## 765	-13.87331810	-0.146656334	0 1143	ThermoMPNN
## 766	-13.85026665	0.062570562	0 1152	ThermoMPNN
## 767	-16.28934879	0.051118306	0 1142	ThermoMPNN
## 768	-14.75866680	0.154577667	0 1148	ThermoMPNN
## 769	-12.88123360	0.493460501	0 1151	ThermoMPNN
## 770	-13.73388824	-0.039668599	0 1153	ThermoMPNN
## 771	-14.28184109	0.279037618	0 1154	ThermoMPNN
## 772	-8.11671715	0.258457260	0 1147	ThermoMPNN
## 773	-13.82312336	-0.121168876	0 1155	ThermoMPNN
## 774	-14.12905178	-0.181807841	0 1156	ThermoMPNN
## 775	-10.58004856	0.334132282	0 1157	ThermoMPNN
## 776	-6.85574093	1.633670601	1 1144	ThermoMPNN
## 777	-16.61373348	-0.169669158	0 1145	ThermoMPNN
## 778	-12.84472542	-0.292759822	0 1146	ThermoMPNN
## 779	-10.82578239	0.909245016	1 1159	ThermoMPNN
## 780	-12.95745144	1.842641810	1 1158	ThermoMPNN
## 781	-14.01627865	0.973112152	1 1168	ThermoMPNN
## 782	-12.76560154	0.574785301	1 1170	ThermoMPNN
## 783	-12.82809696	0.181820467	0 1171	ThermoMPNN
## 784	-12.24641876	0.029955116	0 1173	ThermoMPNN
## 785	-9.12665968	0.001782739	0 1169	ThermoMPNN
## 786	-14.43105412	-0.406604899	0 1164	ThermoMPNN
## 787	-13.92841949	-0.020093982	0 1165	ThermoMPNN
## 788	-12.81098204	-0.035647877	0 1166	ThermoMPNN
## 789	-13.75650234	0.007461112	0 1174	ThermoMPNN
## 790	-16.64490662	-0.221734015	0 1178	ThermoMPNN
## 791	-11.05264797	-0.163457692	0 1175	ThermoMPNN
## 792	-11.19639111	-0.243048962	0 1176	ThermoMPNN
## 793	-10.49650279	-0.283593616	0 1167	ThermoMPNN
## 794	-10.75205588	0.230781251	0 1177	ThermoMPNN
## 795	-15.62361984	0.149154873	0 1162	ThermoMPNN
## 796	-15.43219452	-0.137642521	0 1163	ThermoMPNN
## 797	-10.47761040	0.288154060	0 1160	ThermoMPNN
## 798	-14.10674915	0.396919804	0 1161	ThermoMPNN
## 799	-10.63612747	0.700388634	1 1180	ThermoMPNN
## 800	-13.60583611	0.908791674	1 1181	ThermoMPNN
## 801	-16.49866028	-0.010709968	0 1182	ThermoMPNN
## 802	-16.99456558	0.040626195	0 1183	ThermoMPNN
## 803	-15.64094334	-0.188051691	0 1184	ThermoMPNN
## 804	-14.06229000	-0.181117750	0 1185	ThermoMPNN
## 805	-16.38908501	-0.181220835	0 1186	ThermoMPNN
## 806	-15.11622219	0.104259278	0 1188	ThermoMPNN
## 807	-15.14772358	-0.053818617	0 1189	ThermoMPNN
## 808	-12.54046497	0.056341735	0 1190	ThermoMPNN
## 809	-14.35838223	0.007956292	0 1192	ThermoMPNN
## 810	-16.78042374	-0.119817012	0 1193	ThermoMPNN
## 811	-14.02461662	0.017732478	0 1194	ThermoMPNN
## 812	-7.78168859	0.647770828	1 1195	ThermoMPNN
## 813	-14.28188629	0.360195056	0 1197	ThermoMPNN
## 814	-16.05067024	-0.231710826	0 1198	ThermoMPNN
## 815	-16.44872036	-0.128530070	0 1199	ThermoMPNN

## 816	-15.15670242	-0.128679911	0 1200	ThermoMPNN
## 817	-10.15058556	-0.201220119	0 1201	ThermoMPNN
## 818	-14.69428368	0.328409410	0 1202	ThermoMPNN
## 819	-16.55306034	-0.029213470	0 1203	ThermoMPNN
## 820	-3.61604462	0.980216640	1 1204	ThermoMPNN
## 821	-15.33426609	-0.024732259	0 1205	ThermoMPNN
## 822	-9.60514145	0.437609474	0 1206	ThermoMPNN
## 823	-14.00845585	-0.073070674	0 1207	ThermoMPNN
## 824	-17.00427742	0.445479362	0 1208	ThermoMPNN
## 825	-11.60784779	0.013297124	0 1209	ThermoMPNN
## 826	-15.42070160	-0.078263706	0 1210	ThermoMPNN
## 827	-13.65608063	0.031674776	0 1211	ThermoMPNN
## 828	-15.62395668	0.193322947	0 1212	ThermoMPNN
## 829	-14.93683643	-0.372873432	0 1213	ThermoMPNN
## 830	-13.77542667	-0.004926680	0 1214	ThermoMPNN
## 831	-12.48132687	0.191419441	0 1215	ThermoMPNN
## 832	-15.59737396	0.198444693	0 1216	ThermoMPNN
## 833	-13.08225136	0.089274582	0 1217	ThermoMPNN
## 834	-10.35581408	0.173174822	0 1218	ThermoMPNN
## 835	-11.95422916	0.168582002	0 1220	ThermoMPNN
## 836	-14.72457790	0.262454732	0 1221	ThermoMPNN
## 837	-15.57875347	0.121920951	0 1223	ThermoMPNN
## 838	-14.17200565	0.365119353	0 1224	ThermoMPNN
## 839	-14.53303585	-0.068858683	0 1225	ThermoMPNN
## 840	-17.88001575	0.203875798	0 1226	ThermoMPNN
## 841	-9.79140987	0.646503255	1 1227	ThermoMPNN
## 842	-16.83190155	0.020918289	0 1228	ThermoMPNN
## 843	-12.36793365	2.291268502	1 1229	ThermoMPNN
## 844	-11.55869083	0.971464785	1 1230	ThermoMPNN
## 845	-16.43689995	-0.007879220	0 1231	ThermoMPNN
## 846	-17.38524590	-0.364300995	0 1232	ThermoMPNN
## 847	-17.19267349	0.213967793	0 1233	ThermoMPNN
## 848	-16.32320728	0.019818255	0 1234	ThermoMPNN
## 849	-15.68230019	0.076390260	0 1235	ThermoMPNN
## 850	-14.43436356	0.042428903	0 1236	ThermoMPNN
## 851	-16.65609035	0.182624700	0 1238	ThermoMPNN
## 852	-16.51836452	1.107268704	1 1239	ThermoMPNN
## 853	-13.64438076	1.008963516	1 1240	ThermoMPNN
## 854	-9.45335493	1.244002516	1 1241	ThermoMPNN
## 855	-13.20744267	1.671289144	1 1243	ThermoMPNN
## 856	-12.69640961	0.937523075	1 1244	ThermoMPNN
## 857	-12.19387131	1.595083669	1 1245	ThermoMPNN
## 858	-13.23165827	2.254057223	1 1242	ThermoMPNN
## 859	-12.57048969	2.879929213	1 1251	ThermoMPNN
## 860	-12.39106865	1.106701550	1 1252	ThermoMPNN
## 861	-8.69720888	1.852111215	1 1253	ThermoMPNN
## 862	-11.16158543	1.637587496	1 1255	ThermoMPNN
## 863	-11.53274021	1.771025488	1 1256	ThermoMPNN
## 864	-13.52772846	1.051492944	1 1257	ThermoMPNN
## 865	-9.97328358	1.130072143	1 1258	ThermoMPNN
## 866	-10.93440075	1.816014427	1 1259	ThermoMPNN
## 867	-7.48010368	1.398911146	1 1246	ThermoMPNN
## 868	-13.12969761	0.240042697	0 1247	ThermoMPNN
## 869	-9.84937153	1.478690588	1 1248	ThermoMPNN

## 870	-10.21307220	0.629436038	1 1249	ThermoMPNN
## 871	-11.38672695	1.194291674	1 1250	ThermoMPNN
## 872	-6.64266195	1.696442127	1 1260	ThermoMPNN
## 873	-9.90187092	1.839315313	1 1261	ThermoMPNN
## 874	-9.52847853	1.683030712	1 1262	ThermoMPNN
## 875	-11.30391178	4.478775219	1 1264	ThermoMPNN
## 876	-7.86146517	2.398829434	1 1265	ThermoMPNN
## 877	-11.44789009	2.661011576	1 1266	ThermoMPNN
## 878	-13.73364372	4.208257219	1 1267	ThermoMPNN
## 879	-12.45013485	0.663326938	1 1268	ThermoMPNN
## 880	-11.14190750	3.866718852	1 1269	ThermoMPNN
## 881	-12.70410061	3.036719427	1 1270	ThermoMPNN
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## 884	-12.05625896	1.046715178	1 1273	ThermoMPNN
## 885	-11.00884762	1.496379018	1 1274	ThermoMPNN
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## 887	-11.79212418	3.156993601	1 1277	ThermoMPNN
## 888	-12.77775841	2.466990316	1 1278	ThermoMPNN
## 889	-12.08896732	2.962439680	1 1279	ThermoMPNN
## 890	-9.43067932	1.762479942	1 1280	ThermoMPNN
## 891	-13.72757969	2.432258834	1 1281	ThermoMPNN
## 892	-14.84625664	1.389913456	1 1282	ThermoMPNN
## 893	-14.49465752	0.332541403	0 1283	ThermoMPNN
## 894	-14.31146736	1.632303803	1 1285	ThermoMPNN
## 895	-14.79364796	1.904003743	1 1286	ThermoMPNN
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## 897	-12.52704601	1.576582404	1 1288	ThermoMPNN
## 898	-8.43166714	4.142018247	1 1289	ThermoMPNN
## 899	-8.34475880	3.619295326	1 1290	ThermoMPNN
## 900	-12.12291756	1.905777924	1 1291	ThermoMPNN
## 901	-12.74939804	2.204531879	1 1292	ThermoMPNN
## 902	-13.87499332	2.217275071	1 1293	ThermoMPNN
## 903	-12.57901287	3.640984527	1 1294	ThermoMPNN
## 904	-10.32535305	1.408239256	1 1295	ThermoMPNN
## 905	-8.68902874	0.818765936	1 1297	ThermoMPNN
## 906	-14.12184143	2.809841416	1 1298	ThermoMPNN
## 907	-13.95495605	0.967945877	1 1299	ThermoMPNN
## 908	-15.62571487	1.897571701	1 1307	ThermoMPNN
## 909	-15.54419804	2.722241364	1 1304	ThermoMPNN
## 910	-16.02967777	0.447422292	0 1302	ThermoMPNN
## 911	-15.10126400	1.114271354	1 1308	ThermoMPNN
## 912	-15.09605122	1.964355780	1 1305	ThermoMPNN
## 913	-13.19356537	0.348763990	0 1306	ThermoMPNN
## 914	-14.24783897	0.896527531	1 1317	ThermoMPNN
## 915	-14.89925194	0.351352672	0 1303	ThermoMPNN
## 916	-10.79744625	1.701297172	1 1315	ThermoMPNN
## 917	-12.98794727	1.165843461	1 1316	ThermoMPNN
## 918	-10.30770988	1.660117281	1 1309	ThermoMPNN
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## 923	-13.18003292	1.223887069	1 1314	ThermoMPNN

## 924	-11.37893162	1.461431364	1 1300	ThermoMPNN
## 925	-15.45023327	1.715357341	1 1310	ThermoMPNN
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## 927	-14.30011520	2.549814461	1 1338	ThermoMPNN
## 928	-10.19457922	2.800840403	1 1336	ThermoMPNN
## 929	-7.93135777	0.668916132	1 1333	ThermoMPNN
## 930	-9.09403343	0.806370574	1 1325	ThermoMPNN
## 931	-9.73395872	0.976969280	1 1320	ThermoMPNN
## 932	-9.81890621	2.900649387	1 1335	ThermoMPNN
## 933	-13.08961964	2.535053084	1 1332	ThermoMPNN
## 934	-9.45235100	0.089933557	0 1326	ThermoMPNN
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## 937	-12.69923401	2.065471461	1 1324	ThermoMPNN
## 938	-7.78404169	0.606123472	1 1331	ThermoMPNN
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## 940	-10.61212158	1.679605981	1 1334	ThermoMPNN
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## 942	-9.01078053	2.313417392	1 1328	ThermoMPNN
## 943	-4.18147974	0.480554772	0 1322	ThermoMPNN
## 944	-12.16431751	0.195508426	0 1321	ThermoMPNN
## 945	-13.58702679	1.241616306	1 1351	ThermoMPNN
## 946	-14.85312386	0.716754217	1 1353	ThermoMPNN
## 947	-17.30724220	2.603763002	1 1352	ThermoMPNN
## 948	-11.41490993	1.472280659	1 1355	ThermoMPNN
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## 950	-14.55770149	2.072377396	1 1346	ThermoMPNN
## 951	-10.91888351	2.692518068	1 1354	ThermoMPNN
## 952	-14.23283749	0.127778681	0 1358	ThermoMPNN
## 953	-14.33985004	2.499358573	1 1348	ThermoMPNN
## 954	-15.11882076	1.673660535	1 1356	ThermoMPNN
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## 956	-16.40903759	0.858723743	1 1359	ThermoMPNN
## 957	-15.74776592	1.790579795	1 1350	ThermoMPNN
## 958	-15.19199963	1.367381097	1 1349	ThermoMPNN
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## 960	-12.75464687	1.663313412	1 1341	ThermoMPNN
## 961	-12.07929726	0.819827645	1 1340	ThermoMPNN
## 962	-11.98901978	1.284322658	1 1343	ThermoMPNN
## 963	-9.17111015	0.849678001	1 1360	ThermoMPNN
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## 965	-10.78681488	1.204006263	1 1362	ThermoMPNN
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## 969	-9.98114071	1.407839627	1 1366	ThermoMPNN
## 970	-11.69901714	0.523504410	0 1367	ThermoMPNN
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## 977	-8.95765982	2.253955328	1 1374	ThermoMPNN

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## 982	-17.50306759	2.059715927	1 1398	ThermoMPNN
## 983	-17.43535728	1.376236449	1 1384	ThermoMPNN
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## 986	-15.63916302	1.367207718	1 1396	ThermoMPNN
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## 989	-17.43464928	0.720177871	1 1381	ThermoMPNN
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## 991	-13.25913219	0.830519932	1 1380	ThermoMPNN
## 992	-14.56547184	0.429246143	0 1394	ThermoMPNN
## 993	-11.60388203	0.792558122	1 1393	ThermoMPNN
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## 998	-14.71065063	0.649337604	1 1391	ThermoMPNN
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## 1001	-10.57461348	2.575539401	1 1401	ThermoMPNN
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## 1007	-6.31580009	2.879028439	1 1408	ThermoMPNN
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## 1009	-7.19391451	1.488678292	1 1410	ThermoMPNN
## 1010	-8.84263096	2.356440552	1 1411	ThermoMPNN
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## 1013	-7.35059156	3.502816918	1 1414	ThermoMPNN
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## 1016	-12.13147221	2.161493555	1 1418	ThermoMPNN
## 1017	-10.99649105	1.132557203	1 1419	ThermoMPNN
## 1018	-16.49849186	0.335829640	0 1430	ThermoMPNN
## 1019	-15.66188278	0.315366916	0 1436	ThermoMPNN
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## 1021	-15.70264702	0.324175851	0 1433	ThermoMPNN
## 1022	-16.97258949	-0.078909858	0 1429	ThermoMPNN
## 1023	-12.35155067	0.265295043	0 1435	ThermoMPNN
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## 1030	-17.47641563	0.249978145	0 1427	ThermoMPNN
## 1031	-12.48171635	0.191016670	0 1434	ThermoMPNN

## 1032	-17.30366135	-0.501517905	0 1424	ThermoMPNN
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## 1034	-13.20929604	0.396485241	0 1422	ThermoMPNN
## 1035	-16.03626728	0.612747645	1 1426	ThermoMPNN
## 1036	-12.08275890	0.256407862	0 1457	ThermoMPNN
## 1037	-11.53818092	1.663712319	1 1455	ThermoMPNN
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## 1039	-14.13637600	2.311256809	1 1441	ThermoMPNN
## 1040	-11.33589649	0.278087490	0 1440	ThermoMPNN
## 1041	-14.30721378	1.230234020	1 1444	ThermoMPNN
## 1042	-12.03951139	2.183450854	1 1459	ThermoMPNN
## 1043	-12.42267132	0.371959969	0 1445	ThermoMPNN
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## 1045	-7.62112293	2.463494001	1 1443	ThermoMPNN
## 1046	-11.17994242	0.728805046	1 1448	ThermoMPNN
## 1047	-13.40017204	0.915738447	1 1454	ThermoMPNN
## 1048	-14.41879406	0.668726479	1 1447	ThermoMPNN
## 1049	-15.66606255	1.833013966	1 1458	ThermoMPNN
## 1050	-13.24444466	0.440939143	0 1450	ThermoMPNN
## 1051	-11.41271696	2.174369108	1 1453	ThermoMPNN
## 1052	-9.07699594	1.948938734	1 1451	ThermoMPNN
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## 1054	-14.21693115	0.589181784	1 1452	ThermoMPNN
## 1055	-18.64026566	1.009471006	1 1462	ThermoMPNN
## 1056	-8.78554621	1.996996880	1 1479	ThermoMPNN
## 1057	-14.86731262	0.753063100	1 1466	ThermoMPNN
## 1058	-14.37256680	0.261013624	0 1477	ThermoMPNN
## 1059	-18.68305817	0.389495120	0 1465	ThermoMPNN
## 1060	-15.36505623	0.535566499	0 1475	ThermoMPNN
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## 1062	-20.52437553	-0.207860038	0 1463	ThermoMPNN
## 1063	-18.89884872	0.500397989	0 1476	ThermoMPNN
## 1064	-19.21274529	0.349344583	0 1473	ThermoMPNN
## 1065	-17.82089233	1.909676864	1 1474	ThermoMPNN
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## 1069	-16.29938011	0.413638998	0 1470	ThermoMPNN
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## 1071	-15.18024864	0.195117114	0 1478	ThermoMPNN
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## 1073	-11.88235683	0.689784258	1 1469	ThermoMPNN
## 1074	-15.01611423	-0.093272328	0 1486	ThermoMPNN
## 1075	-11.40566673	1.583789374	1 1487	ThermoMPNN
## 1076	-18.33048744	0.349420619	0 1483	ThermoMPNN
## 1077	-10.30116482	0.488581342	0 1484	ThermoMPNN
## 1078	-18.12291870	-0.077249335	0 1488	ThermoMPNN
## 1079	-16.11159496	1.902324266	1 1480	ThermoMPNN
## 1080	-10.90867290	1.731026838	1 1490	ThermoMPNN
## 1081	-17.05426502	0.660745853	1 1485	ThermoMPNN
## 1082	-18.29981804	0.207462486	0 1482	ThermoMPNN
## 1083	-14.82342319	0.560311215	0 1492	ThermoMPNN
## 1084	-16.68954659	0.719978970	1 1496	ThermoMPNN
## 1085	-12.22968616	1.182342431	1 1497	ThermoMPNN

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## 1087	-11.21732655	0.042623001	0 1499	ThermoMPNN
## 1088	-14.60386925	1.010474467	1 1481	ThermoMPNN
## 1089	-15.50852146	-0.084153393	0 1493	ThermoMPNN
## 1090	-15.67508564	0.103465245	0 1494	ThermoMPNN
## 1091	-16.16562481	-0.050945178	0 1498	ThermoMPNN
## 1092	-15.61949654	0.730747627	1 1495	ThermoMPNN
## 1093	0.07387457	0.892621936	1 1500	ThermoMPNN
## 1094	-8.98264399	0.075272293	0 1501	ThermoMPNN
## 1095	-11.70741329	0.024382203	0 1502	ThermoMPNN
## 1096	-12.06392889	-0.006017823	0 1503	ThermoMPNN
## 1097	-12.09208775	-0.024810228	0 1504	ThermoMPNN
## 1098	-6.80740719	2.515453626	1 1505	ThermoMPNN
## 1099	-14.35438042	0.066073652	0 1506	ThermoMPNN
## 1100	-14.58296490	0.013914193	0 1508	ThermoMPNN
## 1101	-11.19776545	0.040725725	0 1509	ThermoMPNN
## 1102	-11.18032084	-0.262030843	0 1510	ThermoMPNN
## 1103	-13.05016232	-0.098835399	0 1511	ThermoMPNN
## 1104	-10.79297295	0.051575971	0 1512	ThermoMPNN
## 1105	-14.20974274	0.064746009	0 1513	ThermoMPNN
## 1106	-13.38204498	0.074403174	0 1514	ThermoMPNN
## 1107	-7.32237539	0.005663282	0 1516	ThermoMPNN
## 1108	-8.30846148	0.043276574	0 1517	ThermoMPNN
## 1109	-13.87863159	0.150725332	0 1518	ThermoMPNN
## 1110	-13.56224117	0.047684688	0 1519	ThermoMPNN
## 1111	-18.60990868	0.125938518	0 1522	ThermoMPNN
## 1112	-11.47143955	0.193717546	0 1524	ThermoMPNN
## 1113	-16.42080898	-0.015225475	0 1525	ThermoMPNN
## 1114	-15.09148769	-0.078632711	0 1521	ThermoMPNN
## 1115	-17.24461937	-0.147024834	0 1526	ThermoMPNN
## 1116	-17.58791771	0.419995149	0 1523	ThermoMPNN
## 1117	-16.21178246	-0.039682548	0 1535	ThermoMPNN
## 1118	-15.86083050	0.015475235	0 1536	ThermoMPNN
## 1119	-14.45039272	-0.253830058	0 1532	ThermoMPNN
## 1120	-15.50959110	-0.125057506	0 1533	ThermoMPNN
## 1121	-16.19155121	-0.143237447	0 1534	ThermoMPNN
## 1122	-14.88655643	0.240688075	0 1520	ThermoMPNN
## 1123	-18.93903694	0.003743818	0 1531	ThermoMPNN
## 1124	-9.36979046	0.171665434	0 1537	ThermoMPNN
## 1125	-15.95303879	-0.142665025	0 1538	ThermoMPNN
## 1126	-17.89391575	-0.226898337	0 1539	ThermoMPNN
## 1127	-8.73563023	-0.137564971	0 1530	ThermoMPNN
## 1128	-9.72268248	0.017223795	0 1527	ThermoMPNN
## 1129	-17.40252037	-0.021842011	0 1528	ThermoMPNN
## 1130	-9.89386292	0.003563138	0 1700	ThermoMPNN
## 1131	-13.33414087	-0.045131338	0 1701	ThermoMPNN
## 1132	-17.38337479	0.391292056	0 1702	ThermoMPNN
## 1133	-15.57467957	-0.168328257	0 1703	ThermoMPNN
## 1134	-13.98553257	0.367827061	0 1704	ThermoMPNN
## 1135	-14.60188503	0.051233335	0 1705	ThermoMPNN
## 1136	-19.60562897	-0.109486416	0 1706	ThermoMPNN
## 1137	-8.46580677	0.833788987	1 1707	ThermoMPNN
## 1138	-17.62575359	-0.270337513	0 1708	ThermoMPNN
## 1139	-10.94817829	0.188095076	0 1709	ThermoMPNN

## 1140	-11.10757351	0.044499472	0 1710	ThermoMPNN
## 1141	-17.84064331	-0.117155304	0 1711	ThermoMPNN
## 1142	-17.48809948	0.075417608	0 1712	ThermoMPNN
## 1143	-18.80771408	-0.160442796	0 1713	ThermoMPNN
## 1144	-18.01839848	-0.103769484	0 1714	ThermoMPNN
## 1145	-15.11517029	-0.142164850	0 1715	ThermoMPNN
## 1146	-13.21152782	0.320679765	0 1716	ThermoMPNN
## 1147	-18.93848343	-0.163571377	0 1718	ThermoMPNN
## 1148	-18.27640038	0.022925373	0 1719	ThermoMPNN
## 1149	-12.96892185	2.623700655	1 1739	ThermoMPNN
## 1150	-7.49413471	0.341014429	0 1737	ThermoMPNN
## 1151	-13.38184109	-0.124971255	0 1738	ThermoMPNN
## 1152	-11.42611179	0.722463190	1 1720	ThermoMPNN
## 1153	-12.38674698	0.953005524	1 1721	ThermoMPNN
## 1154	-17.07576065	-0.128777341	0 1722	ThermoMPNN
## 1155	-13.94232063	0.065329875	0 1723	ThermoMPNN
## 1156	-9.12547169	1.848755178	1 1724	ThermoMPNN
## 1157	-11.92723866	0.314781889	0 1734	ThermoMPNN
## 1158	-12.93296928	0.467105524	0 1735	ThermoMPNN
## 1159	-10.92311306	0.691729088	1 1736	ThermoMPNN
## 1160	-6.88432217	0.294456724	0 1727	ThermoMPNN
## 1161	-11.55148716	-0.387249715	0 1733	ThermoMPNN
## 1162	-14.35157738	0.361424623	0 1725	ThermoMPNN
## 1163	-11.82665548	2.225144774	1 1726	ThermoMPNN
## 1164	-13.97520733	0.521277044	0 1732	ThermoMPNN
## 1165	-15.23996124	0.412702660	0 1731	ThermoMPNN
## 1166	-1.88606367	-0.008101269	0 1729	ThermoMPNN
## 1167	-14.03697529	1.133911261	1 1748	ThermoMPNN
## 1168	-13.68610172	0.527097931	0 1745	ThermoMPNN
## 1169	-11.11228104	-0.185741322	0 1747	ThermoMPNN
## 1170	-12.27762642	0.122083984	0 1743	ThermoMPNN
## 1171	-9.59384956	0.442686209	0 1744	ThermoMPNN
## 1172	-9.09657879	2.100703129	1 1746	ThermoMPNN
## 1173	-16.00629711	0.030692722	0 1742	ThermoMPNN
## 1174	-13.40949326	0.430534960	0 1756	ThermoMPNN
## 1175	-9.81225510	0.656789734	1 1757	ThermoMPNN
## 1176	-11.22616730	0.849670622	1 1759	ThermoMPNN
## 1177	-12.24290009	0.330262988	0 1740	ThermoMPNN
## 1178	-10.86237755	0.766568031	1 1741	ThermoMPNN
## 1179	-9.31253033	0.331063825	0 1750	ThermoMPNN
## 1180	-11.50931015	1.877547656	1 1758	ThermoMPNN
## 1181	-12.70903988	-0.005235702	0 1752	ThermoMPNN
## 1182	-11.19001102	0.264968155	0 1755	ThermoMPNN
## 1183	-8.79902420	0.732903061	1 1754	ThermoMPNN
## 1184	-14.30567322	1.019808334	1 1751	ThermoMPNN
## 1185	-11.11622982	1.353403290	1 1760	ThermoMPNN
## 1186	-13.02518539	1.968590658	1 1761	ThermoMPNN
## 1187	-15.18329525	-0.071366075	0 1763	ThermoMPNN
## 1188	-11.99659729	0.335375398	0 1764	ThermoMPNN
## 1189	-14.50513172	-0.173228701	0 1765	ThermoMPNN
## 1190	-16.37865639	-0.119915630	0 1766	ThermoMPNN
## 1191	-6.25591125	0.255482083	0 1767	ThermoMPNN
## 1192	-16.50101147	0.099167300	0 1768	ThermoMPNN
## 1193	-9.84361038	2.232931018	1 1769	ThermoMPNN

## 1194	-9.48668718	1.173644910	1 1770	ThermoMPNN
## 1195	-16.59879646	0.230214326	0 1771	ThermoMPNN
## 1196	-17.71393967	-0.266152794	0 1772	ThermoMPNN
## 1197	-16.17991180	0.064347005	0 1773	ThermoMPNN
## 1198	-15.91553116	0.198614797	0 1774	ThermoMPNN
## 1199	-14.88375797	0.631641749	1 1775	ThermoMPNN
## 1200	-12.96530247	0.840575743	1 1776	ThermoMPNN
## 1201	-15.04631042	-0.045565110	0 1778	ThermoMPNN
## 1202	-15.12865067	-0.172487739	0 1779	ThermoMPNN
## 1203	-8.19246674	2.031958653	1 1783	ThermoMPNN
## 1204	-11.30762405	1.357713758	1 1781	ThermoMPNN
## 1205	-9.00277014	2.543209864	1 1786	ThermoMPNN
## 1206	-12.78015003	0.202848969	0 1799	ThermoMPNN
## 1207	-9.99552536	1.167151851	1 1785	ThermoMPNN
## 1208	-8.14299116	2.587320488	1 1791	ThermoMPNN
## 1209	-13.88775482	0.955852359	1 1784	ThermoMPNN
## 1210	-11.25941658	0.863077682	1 1782	ThermoMPNN
## 1211	-11.01700096	1.279175808	1 1798	ThermoMPNN
## 1212	-7.03852520	2.693821349	1 1796	ThermoMPNN
## 1213	-5.95611391	1.843798047	1 1794	ThermoMPNN
## 1214	-11.51461220	1.378384872	1 1797	ThermoMPNN
## 1215	-11.32533569	0.137704039	0 1789	ThermoMPNN
## 1216	-10.33070335	1.283837407	1 1790	ThermoMPNN
## 1217	-6.62150745	2.302609676	1 1793	ThermoMPNN
## 1218	-11.36841373	0.566008840	1 1787	ThermoMPNN
## 1219	-10.54666471	1.576267656	1 1780	ThermoMPNN
## 1220	-8.95425510	2.608238511	1 1795	ThermoMPNN
## 1221	-14.54573841	-0.094103362	0 1792	ThermoMPNN
## 1222	-9.46803217	0.936851146	1 1800	ThermoMPNN
## 1223	-15.84968204	0.491247519	0 1801	ThermoMPNN
## 1224	-16.66974125	-0.036423342	0 1802	ThermoMPNN
## 1225	-14.70745583	0.032559337	0 1803	ThermoMPNN
## 1226	-12.37356529	1.515034871	1 1804	ThermoMPNN
## 1227	-14.77851486	0.187107803	0 1805	ThermoMPNN
## 1228	-16.92794571	-0.124316817	0 1806	ThermoMPNN
## 1229	-7.04267845	2.057787496	1 1807	ThermoMPNN
## 1230	-15.93865585	0.884842560	1 1808	ThermoMPNN
## 1231	-7.53256893	3.047309466	1 1809	ThermoMPNN
## 1232	-10.02743816	1.196008023	1 1810	ThermoMPNN
## 1233	-16.85005589	0.067954630	0 1811	ThermoMPNN
## 1234	-13.01905575	0.257228773	0 1812	ThermoMPNN
## 1235	-15.70120220	0.424371129	0 1813	ThermoMPNN
## 1236	-15.71897945	0.700031203	1 1814	ThermoMPNN
## 1237	-14.91928291	0.443488593	0 1815	ThermoMPNN
## 1238	-11.55228806	0.457588826	0 1816	ThermoMPNN
## 1239	-16.54337044	0.138356829	0 1818	ThermoMPNN
## 1240	-17.07047787	0.513393914	0 1819	ThermoMPNN
## 1241	-10.01179733	0.044781008	0 1836	ThermoMPNN
## 1242	-9.83817844	0.772389936	1 1822	ThermoMPNN
## 1243	-9.17805882	0.803843386	1 1823	ThermoMPNN
## 1244	-8.72553225	1.563113602	1 1834	ThermoMPNN
## 1245	-10.59126415	0.336499123	0 1821	ThermoMPNN
## 1246	-11.99239140	0.047255346	0 1827	ThermoMPNN
## 1247	-10.54887924	0.411077192	0 1829	ThermoMPNN

## 1248	-10.04168911	0.019661190	0 1833	ThermoMPNN
## 1249	-9.70561924	0.241711286	0 1826	ThermoMPNN
## 1250	-11.35929508	1.552021783	1 1838	ThermoMPNN
## 1251	-9.10841370	1.018792972	1 1835	ThermoMPNN
## 1252	-12.56756592	1.009191385	1 1832	ThermoMPNN
## 1253	-12.52158089	0.685549637	1 1824	ThermoMPNN
## 1254	-12.10585880	0.514565948	0 1839	ThermoMPNN
## 1255	-10.64554157	0.360362730	0 1837	ThermoMPNN
## 1256	-9.98198957	0.192845695	0 1831	ThermoMPNN
## 1257	-11.46102276	0.348658130	0 1830	ThermoMPNN
## 1258	-9.17045498	0.989493483	1 1820	ThermoMPNN
## 1259	-14.71370678	0.361172821	0 1858	ThermoMPNN
## 1260	-6.09815826	0.986687306	1 1842	ThermoMPNN
## 1261	-10.33257809	0.356473563	0 1857	ThermoMPNN
## 1262	-11.87692833	0.755711726	1 1849	ThermoMPNN
## 1263	-10.73766747	1.202666696	1 1846	ThermoMPNN
## 1264	-13.50401421	0.625408351	1 1859	ThermoMPNN
## 1265	-9.04269781	-0.128516267	0 1848	ThermoMPNN
## 1266	-7.82132053	1.038397790	1 1845	ThermoMPNN
## 1267	-10.78181219	0.651166197	1 1855	ThermoMPNN
## 1268	-14.43335152	0.437222441	0 1844	ThermoMPNN
## 1269	-11.33312225	0.451423609	0 1856	ThermoMPNN
## 1270	-9.25046377	0.414920645	0 1840	ThermoMPNN
## 1271	-10.60210762	0.548653397	0 1854	ThermoMPNN
## 1272	-12.65467091	1.108097064	1 1850	ThermoMPNN
## 1273	-12.83182468	0.553963945	0 1847	ThermoMPNN
## 1274	-13.48598289	2.151977073	1 1841	ThermoMPNN
## 1275	-10.28210058	0.553749117	0 1851	ThermoMPNN
## 1276	-8.93873491	0.707268403	1 1853	ThermoMPNN
## 1277	-10.90734005	1.859033057	1 1852	ThermoMPNN
## 1278	-8.19290943	1.044322299	1 1861	ThermoMPNN
## 1279	-9.25288773	0.167645853	0 1879	ThermoMPNN
## 1280	-9.93274708	0.747658572	1 1878	ThermoMPNN
## 1281	-10.52491665	0.498853338	0 1864	ThermoMPNN
## 1282	-9.26389647	1.254488964	1 1867	ThermoMPNN
## 1283	-3.95765946	1.645492365	1 1868	ThermoMPNN
## 1284	-7.24442015	1.352608610	1 1877	ThermoMPNN
## 1285	-3.52894917	0.721382579	1 1862	ThermoMPNN
## 1286	-3.09234986	1.159413914	1 1863	ThermoMPNN
## 1287	-8.12068567	1.364662761	1 1870	ThermoMPNN
## 1288	-6.78898382	0.871346796	1 1876	ThermoMPNN
## 1289	-5.96197672	0.731700675	1 1860	ThermoMPNN
## 1290	-8.17400951	1.298508619	1 1869	ThermoMPNN
## 1291	-8.35059366	2.339607772	1 1872	ThermoMPNN
## 1292	-4.95133889	1.027972219	1 1874	ThermoMPNN
## 1293	-6.12343807	0.652856595	1 1875	ThermoMPNN
## 1294	-4.74019098	0.668055539	1 1873	ThermoMPNN
## 1295	-4.76518393	-0.231492269	0 1871	ThermoMPNN
## 1296	-6.81213465	0.367128170	0 1888	ThermoMPNN
## 1297	-13.15996323	0.886932763	1 1899	ThermoMPNN
## 1298	-6.20530729	1.004734260	1 1882	ThermoMPNN
## 1299	-8.26301184	0.933787358	1 1880	ThermoMPNN
## 1300	-13.67661209	1.059663845	1 1884	ThermoMPNN
## 1301	-11.41006680	0.680010138	1 1887	ThermoMPNN

## 1302	-10.12300320	0.908493733	1 1886	ThermoMPNN
## 1303	-10.72079506	0.854551016	1 1889	ThermoMPNN
## 1304	-13.62749577	0.660629252	1 1898	ThermoMPNN
## 1305	-9.71208305	0.781912300	1 1896	ThermoMPNN
## 1306	-12.62481976	0.738879096	1 1881	ThermoMPNN
## 1307	-10.81295891	0.885076423	1 1890	ThermoMPNN
## 1308	-9.40055399	0.439764048	0 1891	ThermoMPNN
## 1309	-7.67714643	1.145029065	1 1885	ThermoMPNN
## 1310	-8.70942307	0.641462258	1 1894	ThermoMPNN
## 1311	-9.74866657	1.212806258	1 1895	ThermoMPNN
## 1312	-7.20504436	1.309078802	1 1893	ThermoMPNN
## 1313	-8.94513168	0.752027786	1 1897	ThermoMPNN
## 1314	-9.97462540	0.603299170	1 1892	ThermoMPNN
## 1315	-11.91049595	1.071531084	1 1919	ThermoMPNN
## 1316	-11.43987885	1.221177219	1 1901	ThermoMPNN
## 1317	-8.25982952	0.975269272	1 1912	ThermoMPNN
## 1318	-10.91319580	1.662564506	1 1907	ThermoMPNN
## 1319	-8.16152258	0.459582019	0 1906	ThermoMPNN
## 1320	-10.16785631	1.067888032	1 1909	ThermoMPNN
## 1321	-4.77933607	1.045853801	1 1902	ThermoMPNN
## 1322	-7.00072498	1.103586747	1 1900	ThermoMPNN
## 1323	-12.66722775	0.333692159	0 1918	ThermoMPNN
## 1324	-12.81985130	0.873147115	1 1904	ThermoMPNN
## 1325	-6.73038936	0.702228448	1 1905	ThermoMPNN
## 1326	-5.76815600	0.214299936	0 1908	ThermoMPNN
## 1327	-7.51902390	1.096200750	1 1911	ThermoMPNN
## 1328	-8.68343515	1.162764102	1 1916	ThermoMPNN
## 1329	-8.29985447	1.147723221	1 1915	ThermoMPNN
## 1330	-6.21037064	0.972789471	1 1913	ThermoMPNN
## 1331	-8.75475903	1.220302571	1 1917	ThermoMPNN
## 1332	-6.99753475	0.723747802	1 1914	ThermoMPNN
## 1333	-10.00854988	1.685772763	1 1910	ThermoMPNN
## 1334	-10.36952209	1.203391240	1 1921	ThermoMPNN
## 1335	-7.32089491	1.164608217	1 1922	ThermoMPNN
## 1336	-11.21707973	1.165601846	1 1929	ThermoMPNN
## 1337	-8.56943464	1.356120508	1 1920	ThermoMPNN
## 1338	-10.92307615	3.333157887	1 1932	ThermoMPNN
## 1339	-7.93168373	0.456849154	0 1928	ThermoMPNN
## 1340	-6.69847298	1.366857252	1 1934	ThermoMPNN
## 1341	-6.72346420	1.199169396	1 1923	ThermoMPNN
## 1342	-8.87155609	0.017661468	0 1931	ThermoMPNN
## 1343	-8.12923937	1.631783363	1 1933	ThermoMPNN
## 1344	-12.95705147	0.570957790	1 1939	ThermoMPNN
## 1345	-11.83041744	1.251457656	1 1938	ThermoMPNN
## 1346	-8.33927765	1.313858413	1 1935	ThermoMPNN
## 1347	-12.69469910	0.898832542	1 1927	ThermoMPNN
## 1348	-9.21839790	0.572902405	1 1926	ThermoMPNN
## 1349	-10.28278770	1.188270400	1 1936	ThermoMPNN
## 1350	-13.31900063	0.436608257	0 1924	ThermoMPNN
## 1351	-10.70122766	1.105224221	1 1937	ThermoMPNN
## 1352	-7.18088875	1.201833897	1 1946	ThermoMPNN
## 1353	-11.44096470	0.746766858	1 1947	ThermoMPNN
## 1354	-9.57639484	0.587588454	1 1949	ThermoMPNN
## 1355	-10.44191418	0.705106651	1 1950	ThermoMPNN

## 1356	-8.57179899	1.219270434	1 1951	ThermoMPNN
## 1357	-6.43365898	1.287436991	1 1948	ThermoMPNN
## 1358	-12.43030891	0.544885182	0 1958	ThermoMPNN
## 1359	-12.03133202	0.048477899	0 1959	ThermoMPNN
## 1360	-7.73737755	1.397981605	1 1945	ThermoMPNN
## 1361	-9.68411942	1.395001069	1 1956	ThermoMPNN
## 1362	-9.98213730	0.062051255	0 1952	ThermoMPNN
## 1363	-6.78194599	1.283807276	1 1954	ThermoMPNN
## 1364	-8.63049908	0.724947466	1 1955	ThermoMPNN
## 1365	-10.31169281	0.473103852	0 1957	ThermoMPNN
## 1366	-5.93765707	0.880278745	1 1943	ThermoMPNN
## 1367	-12.49472237	0.197898767	0 1944	ThermoMPNN
## 1368	-9.64509153	1.210304661	1 1940	ThermoMPNN
## 1369	-10.20653000	1.168523982	1 1941	ThermoMPNN
## 1370	-8.49662552	0.377371115	0 1942	ThermoMPNN
## 1371	-11.39115629	3.025890098	1 1960	ThermoMPNN
## 1372	-7.89120917	2.219948833	1 1961	ThermoMPNN
## 1373	-11.77270308	1.341732090	1 1962	ThermoMPNN
## 1374	-11.02081270	1.340522796	1 1963	ThermoMPNN
## 1375	-9.97428637	1.614111271	1 1964	ThermoMPNN
## 1376	-9.57280455	2.747291095	1 1965	ThermoMPNN
## 1377	-9.71793699	1.431887107	1 1966	ThermoMPNN
## 1378	-12.77728939	2.135387590	1 1967	ThermoMPNN
## 1379	-11.05227299	0.495279929	0 1968	ThermoMPNN
## 1380	-9.49564533	2.562596010	1 1969	ThermoMPNN
## 1381	-11.16495190	2.360381065	1 1970	ThermoMPNN
## 1382	-11.91046076	3.931145410	1 1971	ThermoMPNN
## 1383	-10.72925396	0.891228157	1 1972	ThermoMPNN
## 1384	-9.52747068	0.444667805	0 1973	ThermoMPNN
## 1385	-6.80154877	3.105246125	1 1974	ThermoMPNN
## 1386	-9.20071354	2.534718770	1 1975	ThermoMPNN
## 1387	-11.58953495	2.796192777	1 1976	ThermoMPNN
## 1388	-11.22504673	1.800382719	1 1977	ThermoMPNN
## 1389	-10.36897345	1.516253115	1 1979	ThermoMPNN
## 1390	-6.44539566	0.392120466	0 1980	ThermoMPNN
## 1391	-8.46423779	0.460222900	0 1981	ThermoMPNN
## 1392	-5.92977953	1.651679493	1 1982	ThermoMPNN
## 1393	-6.72690125	1.588573355	1 1983	ThermoMPNN
## 1394	-9.66517658	0.105682654	0 1984	ThermoMPNN
## 1395	-6.66038857	0.942164990	1 1985	ThermoMPNN
## 1396	-8.10429487	0.603407890	1 1986	ThermoMPNN
## 1397	-5.35971804	0.852334714	1 1988	ThermoMPNN
## 1398	-8.98414650	0.670653571	1 1989	ThermoMPNN
## 1399	-8.17505264	0.503386373	0 1990	ThermoMPNN
## 1400	-4.09543781	1.021033138	1 1991	ThermoMPNN
## 1401	-9.76453829	0.784025058	1 1992	ThermoMPNN
## 1402	-8.00645189	1.257270467	1 1993	ThermoMPNN
## 1403	-7.31685696	0.930854550	1 1994	ThermoMPNN
## 1404	-4.99351482	0.687551152	1 1996	ThermoMPNN
## 1405	-7.86718683	0.618796069	1 1997	ThermoMPNN
## 1406	-9.98084545	0.829002450	1 1999	ThermoMPNN
## 1407	-9.58222923	1.327114408	1 2000	ThermoMPNN
## 1408	-13.67588501	1.153870332	1 2001	ThermoMPNN
## 1409	-13.54659729	0.588275738	1 2002	ThermoMPNN

## 1410	-12.96297836	0.454144977	0	2003	ThermoMPNN
## 1411	-11.57341328	1.190070127	1	2004	ThermoMPNN
## 1412	-12.48856583	0.891931917	1	2005	ThermoMPNN
## 1413	-14.93985100	0.637354865	1	2006	ThermoMPNN
## 1414	-6.44512186	0.673213365	1	2007	ThermoMPNN
## 1415	-14.09334278	0.412850181	0	2008	ThermoMPNN
## 1416	-10.20093212	0.701679493	1	2009	ThermoMPNN
## 1417	-9.35159073	0.878999215	1	2010	ThermoMPNN
## 1418	-14.39981995	1.263589056	1	2011	ThermoMPNN
## 1419	-13.42027683	0.754023243	1	2012	ThermoMPNN
## 1420	-13.90547543	1.577569747	1	2013	ThermoMPNN
## 1421	-13.59916992	0.562683596	0	2014	ThermoMPNN
## 1422	-12.42296734	0.933960702	1	2015	ThermoMPNN
## 1423	-10.77588692	0.770434104	1	2016	ThermoMPNN
## 1424	-15.66287975	1.377572082	1	2018	ThermoMPNN
## 1425	-14.37363682	0.736079082	1	2019	ThermoMPNN
## 1426	-12.59400311	0.180922237	0	2024	ThermoMPNN
## 1427	-6.60144186	1.874075459	1	2022	ThermoMPNN
## 1428	-5.15967894	0.954391156	1	2023	ThermoMPNN
## 1429	-9.22037992	0.930025923	1	2035	ThermoMPNN
## 1430	-9.87265568	0.797810968	1	2025	ThermoMPNN
## 1431	-11.93454533	0.204910196	0	2021	ThermoMPNN
## 1432	-9.31193104	0.886354449	1	2020	ThermoMPNN
## 1433	-7.87145443	1.048927764	1	2036	ThermoMPNN
## 1434	-7.95429535	0.304666196	0	2037	ThermoMPNN
## 1435	-12.01793690	0.510482730	0	2039	ThermoMPNN
## 1436	-13.69687080	-0.147222060	0	2038	ThermoMPNN
## 1437	-7.50874043	0.606738826	1	2034	ThermoMPNN
## 1438	-9.41924772	-0.188987841	0	2026	ThermoMPNN
## 1439	-7.44943514	-0.107314407	0	2027	ThermoMPNN
## 1440	-7.05238342	1.622560195	1	2033	ThermoMPNN
## 1441	-13.07808819	0.126322663	0	2032	ThermoMPNN
## 1442	-10.13215370	1.321766760	1	2029	ThermoMPNN
## 1443	-9.24890099	0.699994309	1	2040	ThermoMPNN
## 1444	-13.34071665	0.526528582	0	2041	ThermoMPNN
## 1445	-12.81116028	1.043687091	1	2042	ThermoMPNN
## 1446	-12.45952740	1.392252782	1	2043	ThermoMPNN
## 1447	-13.76578178	-0.092455803	0	2044	ThermoMPNN
## 1448	-12.61035242	0.619201660	1	2045	ThermoMPNN
## 1449	-13.32690401	0.854770012	1	2046	ThermoMPNN
## 1450	-8.78402643	-0.047349750	0	2047	ThermoMPNN
## 1451	-11.63488178	-0.044229352	0	2048	ThermoMPNN
## 1452	-11.54516630	0.091463154	0	2049	ThermoMPNN
## 1453	-8.47950950	0.278854649	0	2050	ThermoMPNN
## 1454	-10.25005894	0.591681886	1	2051	ThermoMPNN
## 1455	-12.92245922	0.846122356	1	2052	ThermoMPNN
## 1456	-11.85913477	0.215487703	0	2053	ThermoMPNN
## 1457	-12.68761635	0.262925466	0	2054	ThermoMPNN
## 1458	-8.25817518	1.661292019	1	2055	ThermoMPNN
## 1459	-10.70533371	-0.036477397	0	2057	ThermoMPNN
## 1460	-16.13659477	0.394421262	0	2058	ThermoMPNN
## 1461	-13.94484177	0.471321530	0	2059	ThermoMPNN
## 1462	-10.98186207	1.270633594	1	2067	ThermoMPNN
## 1463	-13.21068554	1.341667797	1	2069	ThermoMPNN

## 1464	-11.41572847	0.722786060	1	2066	ThermoMPNN
## 1465	-14.89667568	1.401493560	1	2078	ThermoMPNN
## 1466	-11.47202339	0.722166675	1	2070	ThermoMPNN
## 1467	-12.42214508	0.608974596	1	2060	ThermoMPNN
## 1468	-9.89600611	0.437667261	0	2071	ThermoMPNN
## 1469	-8.58887644	0.488788533	0	2063	ThermoMPNN
## 1470	-13.76007919	0.997289854	1	2064	ThermoMPNN
## 1471	-11.38600731	1.856366629	1	2062	ThermoMPNN
## 1472	-12.38501854	0.472650145	0	2065	ThermoMPNN
## 1473	-11.87222443	1.133915793	1	2077	ThermoMPNN
## 1474	-13.53591747	1.072581380	1	2061	ThermoMPNN
## 1475	-9.36939259	1.324287827	1	2073	ThermoMPNN
## 1476	-7.89888754	0.894448671	1	2074	ThermoMPNN
## 1477	-12.46060829	0.665412802	1	2079	ThermoMPNN
## 1478	-9.60810184	1.161969105	1	2076	ThermoMPNN
## 1479	-15.10394993	0.188091283	0	2072	ThermoMPNN
## 1480	-11.29585199	0.964570319	1	2075	ThermoMPNN
## 1481	-13.56465206	-0.049581754	0	2087	ThermoMPNN
## 1482	-14.95529346	0.280324619	0	2090	ThermoMPNN
## 1483	-13.68074932	0.609714288	1	2092	ThermoMPNN
## 1484	-12.67284946	-0.095441658	0	2088	ThermoMPNN
## 1485	-12.28846340	0.325032294	0	2082	ThermoMPNN
## 1486	-13.60746613	0.836280408	1	2083	ThermoMPNN
## 1487	-10.91360693	0.096886193	0	2081	ThermoMPNN
## 1488	-9.15661840	0.902728648	1	2093	ThermoMPNN
## 1489	-7.62259045	0.353986331	0	2091	ThermoMPNN
## 1490	-11.87601166	1.398290619	1	2085	ThermoMPNN
## 1491	-12.88969631	0.839764907	1	2080	ThermoMPNN
## 1492	-10.92553921	0.592139152	1	2094	ThermoMPNN
## 1493	-11.82611675	0.350916710	0	2089	ThermoMPNN
## 1494	-9.73077126	2.139938518	1	2095	ThermoMPNN
## 1495	-11.18526497	0.649957143	1	2084	ThermoMPNN
## 1496	-15.22310944	0.885404685	1	2098	ThermoMPNN
## 1497	-13.80228977	0.140831695	0	2097	ThermoMPNN
## 1498	-8.65074129	0.926560472	1	2099	ThermoMPNN
## 1499	-12.76776943	0.135958132	0	2096	ThermoMPNN
## 1500	-12.82105160	0.628475012	1	2119	ThermoMPNN
## 1501	-10.13511496	0.430612305	0	2114	ThermoMPNN
## 1502	-11.58002644	0.659960223	1	2117	ThermoMPNN
## 1503	-14.19684067	0.701730738	1	2118	ThermoMPNN
## 1504	-11.43796883	1.065076421	1	2115	ThermoMPNN
## 1505	-12.55302620	0.458693817	0	2116	ThermoMPNN
## 1506	-7.43552046	1.022210856	1	2103	ThermoMPNN
## 1507	-14.08488712	0.432924708	0	2104	ThermoMPNN
## 1508	-11.99982166	0.858682159	1	2100	ThermoMPNN
## 1509	-13.26671867	0.662970345	1	2101	ThermoMPNN
## 1510	-11.76290607	0.881137490	1	2110	ThermoMPNN
## 1511	-12.49320717	1.014283508	1	2111	ThermoMPNN
## 1512	-14.51578636	-0.124848130	0	2112	ThermoMPNN
## 1513	-12.81164112	0.105561366	0	2105	ThermoMPNN
## 1514	-8.35446415	0.426809868	0	2108	ThermoMPNN
## 1515	-11.13805180	0.776622367	1	2109	ThermoMPNN
## 1516	-12.91440105	0.922009869	1	2107	ThermoMPNN
## 1517	-9.59993401	0.774173432	1	2106	ThermoMPNN

## 1518	-9.69479389	-0.052262104	0 2137	ThermoMPNN
## 1519	-10.15765915	0.343548880	0 2136	ThermoMPNN
## 1520	-15.64120045	0.360265247	0 2138	ThermoMPNN
## 1521	-14.82603245	0.223297222	0 2139	ThermoMPNN
## 1522	-12.73982067	0.376176507	0 2123	ThermoMPNN
## 1523	-12.63164330	0.628920857	1 2120	ThermoMPNN
## 1524	-14.51017799	0.383298114	0 2121	ThermoMPNN
## 1525	-15.35642757	0.246582812	0 2122	ThermoMPNN
## 1526	-12.19095001	0.418854285	0 2134	ThermoMPNN
## 1527	-12.90988064	0.477526232	0 2135	ThermoMPNN
## 1528	-16.25883904	1.625694905	1 2132	ThermoMPNN
## 1529	-13.70446110	0.457013341	0 2131	ThermoMPNN
## 1530	-12.34681034	1.053941635	1 2133	ThermoMPNN
## 1531	-15.28725681	1.511445221	1 2125	ThermoMPNN
## 1532	-14.67858219	0.297020447	0 2126	ThermoMPNN
## 1533	-7.26628361	0.599025716	1 2127	ThermoMPNN
## 1534	-13.33578949	0.674704838	1 2124	ThermoMPNN
## 1535	-9.19646053	0.394048452	0 2129	ThermoMPNN
## 1536	-11.18556747	0.187127943	0 2128	ThermoMPNN
## 1537	-16.14341316	0.056347459	0 2140	ThermoMPNN
## 1538	-9.65171280	0.044245118	0 2141	ThermoMPNN
## 1539	-16.04556179	-0.314581582	0 2142	ThermoMPNN
## 1540	-17.32755814	-0.100223579	0 2143	ThermoMPNN
## 1541	-8.03712225	0.612622401	1 2144	ThermoMPNN
## 1542	-16.93078289	0.131824737	0 2145	ThermoMPNN
## 1543	-11.14373894	-0.242656841	0 2146	ThermoMPNN
## 1544	-14.64690971	-0.025756929	0 2147	ThermoMPNN
## 1545	-17.14086170	-0.277791868	0 2148	ThermoMPNN
## 1546	-13.61021366	-0.271792237	0 2149	ThermoMPNN
## 1547	-17.22405720	-0.066953213	0 2150	ThermoMPNN
## 1548	-15.01237602	-0.130100659	0 2151	ThermoMPNN
## 1549	-17.30600281	0.202493618	0 2152	ThermoMPNN
## 1550	-15.86416130	0.019865638	0 2153	ThermoMPNN
## 1551	-15.68513470	-0.060844672	0 2154	ThermoMPNN
## 1552	-13.54522076	-0.055256560	0 2155	ThermoMPNN
## 1553	-16.82297935	-0.047832038	0 2156	ThermoMPNN
## 1554	-13.64352646	-0.287582141	0 2157	ThermoMPNN
## 1555	-15.83154736	-0.332295429	0 2158	ThermoMPNN
## 1556	-7.30791721	0.617659855	1 2160	ThermoMPNN
## 1557	-10.29439907	0.948539602	1 2161	ThermoMPNN
## 1558	-13.43798923	0.144172042	0 2162	ThermoMPNN
## 1559	-14.17791309	0.371799172	0 2163	ThermoMPNN
## 1560	-11.72589188	0.976991434	1 2164	ThermoMPNN
## 1561	-10.98488503	0.166909347	0 2165	ThermoMPNN
## 1562	-12.13773136	0.757926552	1 2166	ThermoMPNN
## 1563	-12.42257042	0.339662270	0 2167	ThermoMPNN
## 1564	-13.24988594	0.790066954	1 2168	ThermoMPNN
## 1565	-10.72607021	0.009151636	0 2169	ThermoMPNN
## 1566	-13.16069050	0.091272516	0 2170	ThermoMPNN
## 1567	-9.78602200	0.564756018	1 2171	ThermoMPNN
## 1568	-9.71479511	-0.256230303	0 2172	ThermoMPNN
## 1569	-13.03692493	0.283101492	0 2173	ThermoMPNN
## 1570	-10.75286312	0.403111774	0 2174	ThermoMPNN
## 1571	-8.96735306	1.372620326	1 2176	ThermoMPNN

## 1572	-12.12352638	0.553674859	0 2177	ThermoMPNN
## 1573	-14.42373505	0.456669157	0 2178	ThermoMPNN
## 1574	-12.72178192	1.130070808	1 2179	ThermoMPNN
## 1575	-17.91838951	-0.037814116	0 2183	ThermoMPNN
## 1576	-18.18460884	-0.187648155	0 2193	ThermoMPNN
## 1577	-19.04541473	-0.322214645	0 2182	ThermoMPNN
## 1578	-16.93278522	0.257794169	0 2191	ThermoMPNN
## 1579	-16.84635620	0.277280268	0 2192	ThermoMPNN
## 1580	-17.57905464	1.104921919	1 2181	ThermoMPNN
## 1581	-11.55803318	0.524419846	0 2190	ThermoMPNN
## 1582	-16.81416531	0.405839718	0 2195	ThermoMPNN
## 1583	-10.98950157	1.176256175	1 2189	ThermoMPNN
## 1584	-19.67151756	-0.088568196	0 2198	ThermoMPNN
## 1585	-17.29539509	-0.096107862	0 2194	ThermoMPNN
## 1586	-18.53776016	-0.363283055	0 2199	ThermoMPNN
## 1587	-9.58442535	0.292688989	0 2197	ThermoMPNN
## 1588	-14.65711308	0.273012128	0 2184	ThermoMPNN
## 1589	-15.28469410	-0.299073372	0 2180	ThermoMPNN
## 1590	-17.32493477	-0.236593438	0 2188	ThermoMPNN
## 1591	-18.22228088	0.258392634	0 2186	ThermoMPNN
## 1592	-17.89371433	0.284664791	0 2185	ThermoMPNN
## 1593	-12.88980064	0.201351712	0 2196	ThermoMPNN
## 1594	-16.39054718	0.230596874	0 2219	ThermoMPNN
## 1595	-9.66589699	0.782474341	1 2215	ThermoMPNN
## 1596	-11.65437946	0.776129681	1 2216	ThermoMPNN
## 1597	-17.24654350	-0.123896252	0 2218	ThermoMPNN
## 1598	-12.24859619	0.665733888	1 2214	ThermoMPNN
## 1599	-15.24658337	1.057481567	1 2201	ThermoMPNN
## 1600	-14.60178680	1.153762956	1 2202	ThermoMPNN
## 1601	-15.48031254	0.174423561	0 2217	ThermoMPNN
## 1602	-11.30115738	0.918814612	1 2200	ThermoMPNN
## 1603	-12.45108852	0.478686715	0 2206	ThermoMPNN
## 1604	-10.82980671	0.259546229	0 2209	ThermoMPNN
## 1605	-15.46881657	0.340485008	0 2210	ThermoMPNN
## 1606	-15.00287933	0.890044626	1 2211	ThermoMPNN
## 1607	-11.63314819	0.670761185	1 2213	ThermoMPNN
## 1608	-13.98960533	0.599232949	1 2205	ThermoMPNN
## 1609	-16.12593327	0.238450118	0 2207	ThermoMPNN
## 1610	-14.22019253	1.137513417	1 2203	ThermoMPNN
## 1611	-16.06902771	0.204194062	0 2204	ThermoMPNN
## 1612	-14.61022072	1.111906914	1 2208	ThermoMPNN
## 1613	-14.57753296	1.711140256	1 2239	ThermoMPNN
## 1614	-11.92278900	1.018806117	1 2236	ThermoMPNN
## 1615	-10.66284142	1.057390263	1 2225	ThermoMPNN
## 1616	-16.07916641	-0.004067935	0 2238	ThermoMPNN
## 1617	-15.36954327	0.808997795	1 2221	ThermoMPNN
## 1618	-15.41876965	0.543480200	0 2224	ThermoMPNN
## 1619	-10.01795092	0.884502528	1 2220	ThermoMPNN
## 1620	-8.69941883	1.017695461	1 2222	ThermoMPNN
## 1621	-11.39987011	1.541721294	1 2237	ThermoMPNN
## 1622	-12.06958923	0.779782561	1 2234	ThermoMPNN
## 1623	-11.42249079	1.018364073	1 2226	ThermoMPNN
## 1624	-12.96658268	1.013061527	1 2227	ThermoMPNN
## 1625	-13.67379093	0.962646481	1 2230	ThermoMPNN

## 1626	-11.36619453	1.009330705	1 2235	ThermoMPNN
## 1627	-8.05250521	1.211674635	1 2233	ThermoMPNN
## 1628	-12.25770359	0.984624342	1 2231	ThermoMPNN
## 1629	-10.05866165	0.571587725	1 2228	ThermoMPNN
## 1630	-10.46019735	0.858419790	1 2232	ThermoMPNN
## 1631	-12.54630833	1.059867249	1 2229	ThermoMPNN
## 1632	-9.84739046	0.826590819	1 2255	ThermoMPNN
## 1633	-14.30346508	0.656729110	1 2250	ThermoMPNN
## 1634	-9.42135010	1.290400969	1 2245	ThermoMPNN
## 1635	-15.40483475	1.058990959	1 2258	ThermoMPNN
## 1636	-8.44550714	0.466177399	0 2251	ThermoMPNN
## 1637	-12.83671818	0.921231072	1 2249	ThermoMPNN
## 1638	-13.77418842	1.110176912	1 2252	ThermoMPNN
## 1639	-12.95337038	0.884055562	1 2244	ThermoMPNN
## 1640	-11.46201925	0.926294824	1 2256	ThermoMPNN
## 1641	-11.14698458	1.054108441	1 2257	ThermoMPNN
## 1642	-12.30943918	1.698193100	1 2248	ThermoMPNN
## 1643	-13.23085861	1.116362638	1 2247	ThermoMPNN
## 1644	-11.03216496	1.319572637	1 2259	ThermoMPNN
## 1645	-6.89055047	1.209287945	1 2243	ThermoMPNN
## 1646	-10.39254303	1.135097972	1 2240	ThermoMPNN
## 1647	-11.41828270	0.641270139	1 2253	ThermoMPNN
## 1648	-13.41015224	1.069218569	1 2254	ThermoMPNN
## 1649	-8.78793478	0.940875423	1 2246	ThermoMPNN
## 1650	-13.26092815	0.731667557	1 2241	ThermoMPNN
## 1651	-13.99230480	1.852450305	1 2268	ThermoMPNN
## 1652	-13.52146397	0.700736234	1 2261	ThermoMPNN
## 1653	-13.37437325	0.785029811	1 2263	ThermoMPNN
## 1654	-10.40067978	1.128742332	1 2276	ThermoMPNN
## 1655	-8.66784458	0.142001617	0 2277	ThermoMPNN
## 1656	-14.72380333	1.572785103	1 2274	ThermoMPNN
## 1657	-9.51299143	1.202979940	1 2275	ThermoMPNN
## 1658	-10.83817520	0.182391983	0 2267	ThermoMPNN
## 1659	-11.62929878	1.519774892	1 2270	ThermoMPNN
## 1660	-14.28355312	1.078610455	1 2266	ThermoMPNN
## 1661	-9.03821163	1.101852440	1 2269	ThermoMPNN
## 1662	-17.06638184	0.788459624	1 2278	ThermoMPNN
## 1663	-11.67321148	0.217804904	0 2265	ThermoMPNN
## 1664	-13.75349674	1.066647931	1 2264	ThermoMPNN
## 1665	-15.17058716	0.892265792	1 2279	ThermoMPNN
## 1666	-12.88530388	0.615039527	1 2272	ThermoMPNN
## 1667	-14.21005764	1.151542443	1 2271	ThermoMPNN
## 1668	-13.59715347	0.475058286	0 2273	ThermoMPNN
## 1669	-17.44992504	-0.086445748	0 2292	ThermoMPNN
## 1670	-14.04129257	0.586992264	1 2293	ThermoMPNN
## 1671	-13.84916553	0.504386647	0 2295	ThermoMPNN
## 1672	-14.31396503	-0.241384896	0 2291	ThermoMPNN
## 1673	-13.17366562	0.167846827	0 2280	ThermoMPNN
## 1674	-11.10253544	1.419273626	1 2294	ThermoMPNN
## 1675	-11.48146801	0.923112535	1 2289	ThermoMPNN
## 1676	-16.87623539	1.716137522	1 2299	ThermoMPNN
## 1677	-15.30874500	0.349165307	0 2284	ThermoMPNN
## 1678	-14.32104301	-0.061346161	0 2285	ThermoMPNN
## 1679	-15.64807167	0.286167508	0 2281	ThermoMPNN

## 1680	-16.82793922	0.003869662	0 2282	ThermoMPNN
## 1681	-17.37802868	-0.108224932	0 2298	ThermoMPNN
## 1682	-14.98819923	0.455145011	0 2283	ThermoMPNN
## 1683	-16.09141560	0.252407236	0 2286	ThermoMPNN
## 1684	-10.37820263	1.271389202	1 2287	ThermoMPNN
## 1685	-11.34807549	0.514330167	0 2297	ThermoMPNN
## 1686	-10.61475525	0.219438837	0 2296	ThermoMPNN
## 1687	-8.90765324	0.549966558	0 2300	ThermoMPNN
## 1688	-11.34137135	0.936182470	1 2301	ThermoMPNN
## 1689	-14.35960941	0.320335660	0 2302	ThermoMPNN
## 1690	-12.22674236	-0.099424053	0 2303	ThermoMPNN
## 1691	-12.04334850	0.492544329	0 2305	ThermoMPNN
## 1692	-10.87961464	0.739113152	1 2306	ThermoMPNN
## 1693	-8.33352785	0.713135176	1 2307	ThermoMPNN
## 1694	-9.89944239	0.467363805	0 2308	ThermoMPNN
## 1695	-7.51933012	0.571668353	1 2309	ThermoMPNN
## 1696	-7.84913931	1.055192845	1 2310	ThermoMPNN
## 1697	-10.53804226	0.692457784	1 2311	ThermoMPNN
## 1698	-13.17629547	-0.233693871	0 2312	ThermoMPNN
## 1699	-9.22764149	0.232463241	0 2313	ThermoMPNN
## 1700	-9.84191895	0.344999107	0 2314	ThermoMPNN
## 1701	-8.28674049	0.675758815	1 2315	ThermoMPNN
## 1702	-8.08906994	1.158272858	1 2317	ThermoMPNN
## 1703	-14.89855843	0.068061673	0 2318	ThermoMPNN
## 1704	-12.83918362	-0.068141653	0 2319	ThermoMPNN
## 1705	-16.06551456	-0.369393753	0 2339	ThermoMPNN
## 1706	-15.66808853	-0.156365144	0 2327	ThermoMPNN
## 1707	-13.82891846	1.267241685	1 2336	ThermoMPNN
## 1708	-14.88929253	0.138363711	0 2329	ThermoMPNN
## 1709	-15.99909439	0.037988078	0 2324	ThermoMPNN
## 1710	-11.29990788	0.119110057	0 2323	ThermoMPNN
## 1711	-14.51334953	0.294951690	0 2328	ThermoMPNN
## 1712	-10.04881325	1.259891618	1 2335	ThermoMPNN
## 1713	-12.15726204	0.633169841	1 2321	ThermoMPNN
## 1714	-14.96781216	0.568243245	1 2326	ThermoMPNN
## 1715	-12.37173195	0.251068654	0 2337	ThermoMPNN
## 1716	-10.34458275	0.371707126	0 2322	ThermoMPNN
## 1717	-11.49653149	0.352065498	0 2334	ThermoMPNN
## 1718	-14.47534618	0.025269964	0 2338	ThermoMPNN
## 1719	-15.36097240	0.368063983	0 2333	ThermoMPNN
## 1720	-10.08250771	0.814034497	1 2320	ThermoMPNN
## 1721	-13.02562981	1.001199720	1 2331	ThermoMPNN
## 1722	-16.13936653	0.077357551	0 2330	ThermoMPNN
## 1723	-15.75876846	0.068467691	0 2332	ThermoMPNN
## 1724	-9.46161461	-0.093876007	0 2340	ThermoMPNN
## 1725	-13.16604691	0.403330500	0 2341	ThermoMPNN
## 1726	-12.84873753	0.195230606	0 2342	ThermoMPNN
## 1727	-13.29465199	-0.053183716	0 2343	ThermoMPNN
## 1728	-15.77753429	-0.250934607	0 2344	ThermoMPNN
## 1729	-11.99913197	0.091112601	0 2345	ThermoMPNN
## 1730	-14.24827919	0.198460527	0 2346	ThermoMPNN
## 1731	-11.91721630	0.045672836	0 2347	ThermoMPNN
## 1732	-14.29584103	-0.002236959	0 2349	ThermoMPNN
## 1733	-12.57121372	-0.074745909	0 2350	ThermoMPNN

## 1734	-10.07267084	-0.128241477	0 2351	ThermoMPNN
## 1735	-11.11890965	-0.519531901	0 2352	ThermoMPNN
## 1736	-14.31256924	0.560329721	0 2353	ThermoMPNN
## 1737	-12.61781216	0.159597486	0 2354	ThermoMPNN
## 1738	-6.86100035	0.886902444	1 2355	ThermoMPNN
## 1739	-13.20903416	0.081890193	0 2357	ThermoMPNN
## 1740	-18.77784843	-0.117710322	0 2358	ThermoMPNN
## 1741	-15.49947548	-0.080966062	0 2359	ThermoMPNN
## 1742	-14.67168083	-0.127911740	0 2367	ThermoMPNN
## 1743	-9.87604237	-0.373883310	0 2372	ThermoMPNN
## 1744	-14.11763420	-0.172921114	0 2371	ThermoMPNN
## 1745	-12.60035496	0.100858911	0 2366	ThermoMPNN
## 1746	-11.34108067	-0.274599710	0 2374	ThermoMPNN
## 1747	-6.84022341	-0.192970873	0 2365	ThermoMPNN
## 1748	-13.95973473	-0.133710047	0 2368	ThermoMPNN
## 1749	-12.33930321	0.116565295	0 2377	ThermoMPNN
## 1750	-14.15786037	-0.149378486	0 2379	ThermoMPNN
## 1751	-13.99211998	-0.105235623	0 2369	ThermoMPNN
## 1752	-13.51309586	1.504786898	1 2373	ThermoMPNN
## 1753	-10.95883427	-0.326926097	0 2376	ThermoMPNN
## 1754	-14.05008907	-0.116657869	0 2362	ThermoMPNN
## 1755	-15.22072506	1.192733979	1 2370	ThermoMPNN
## 1756	-12.40067558	0.238630954	0 2363	ThermoMPNN
## 1757	-5.48427143	0.403730844	0 2375	ThermoMPNN
## 1758	-14.22689724	-0.189011311	0 2364	ThermoMPNN
## 1759	-14.89436283	-0.175359320	0 2378	ThermoMPNN
## 1760	-11.87738247	0.108548245	0 2361	ThermoMPNN
## 1761	-13.01842003	0.485316174	0 2386	ThermoMPNN
## 1762	-10.45925064	1.323236397	1 2380	ThermoMPNN
## 1763	-17.73396111	0.468941547	0 2398	ThermoMPNN
## 1764	-11.33387756	1.310168677	1 2397	ThermoMPNN
## 1765	-12.65513058	-0.366277494	0 2391	ThermoMPNN
## 1766	-13.55825863	-0.121329988	0 2392	ThermoMPNN
## 1767	-13.33060970	0.404366836	0 2389	ThermoMPNN
## 1768	-15.57284908	0.713023698	1 2399	ThermoMPNN
## 1769	-14.03569393	0.831888483	1 2390	ThermoMPNN
## 1770	-8.68223553	0.534234263	0 2382	ThermoMPNN
## 1771	-14.21006737	0.750859022	1 2387	ThermoMPNN
## 1772	-11.86620979	0.748868079	1 2388	ThermoMPNN
## 1773	-11.44047432	0.623011000	1 2385	ThermoMPNN
## 1774	-11.37850094	0.772199123	1 2396	ThermoMPNN
## 1775	-12.00606899	1.025804276	1 2395	ThermoMPNN
## 1776	-9.63905916	1.258079550	1 2393	ThermoMPNN
## 1777	-15.79429245	0.910174808	1 2381	ThermoMPNN
## 1778	-15.95346565	0.083682820	0 2384	ThermoMPNN
## 1779	-14.00677643	0.455106850	0 2394	ThermoMPNN
## 1780	-15.35652027	0.355569908	0 2419	ThermoMPNN
## 1781	-10.21584187	0.856461573	1 2417	ThermoMPNN
## 1782	-16.44765491	0.437434972	0 2418	ThermoMPNN
## 1783	-11.30122776	0.553421383	0 2415	ThermoMPNN
## 1784	-9.80731392	0.588734803	1 2416	ThermoMPNN
## 1785	-13.82559509	0.724051368	1 2404	ThermoMPNN
## 1786	-12.36117725	0.756015334	1 2414	ThermoMPNN
## 1787	-11.66515770	0.828076787	1 2405	ThermoMPNN

## 1788	-14.88297253	1.600633473	1 2401	ThermoMPNN
## 1789	-8.87634726	0.664962925	1 2403	ThermoMPNN
## 1790	-14.17676678	0.005910382	0 2412	ThermoMPNN
## 1791	-8.70562592	1.201463415	1 2400	ThermoMPNN
## 1792	-10.41252346	0.270136410	0 2407	ThermoMPNN
## 1793	-10.46109314	0.185670140	0 2402	ThermoMPNN
## 1794	-9.68209782	0.442090122	0 2413	ThermoMPNN
## 1795	-12.89463673	0.464014370	0 2406	ThermoMPNN
## 1796	-9.91623726	0.249524243	0 2408	ThermoMPNN
## 1797	-10.55646687	0.228381603	0 2409	ThermoMPNN
## 1798	-12.03953075	0.620220940	1 2411	ThermoMPNN
## 1799	-18.00198135	0.496641044	0 2434	ThermoMPNN
## 1800	-15.96117496	-0.129288114	0 2435	ThermoMPNN
## 1801	-17.09876709	0.124523023	0 2421	ThermoMPNN
## 1802	-16.47365456	0.046511839	0 2436	ThermoMPNN
## 1803	-19.08219719	-0.066219133	0 2425	ThermoMPNN
## 1804	-20.04212456	-0.294819404	0 2422	ThermoMPNN
## 1805	-16.60633354	-0.206104947	0 2433	ThermoMPNN
## 1806	-17.95340748	-0.094737843	0 2426	ThermoMPNN
## 1807	-16.46599770	-0.174221076	0 2420	ThermoMPNN
## 1808	-12.90202885	0.449024602	0 2427	ThermoMPNN
## 1809	-18.40170059	-0.368923993	0 2423	ThermoMPNN
## 1810	-12.35984116	-0.339734481	0 2424	ThermoMPNN
## 1811	-18.99927368	-0.239161931	0 2438	ThermoMPNN
## 1812	-17.87211571	0.397904225	0 2439	ThermoMPNN
## 1813	-12.27163239	-0.118341358	0 2437	ThermoMPNN
## 1814	-19.28504219	-0.274676841	0 2431	ThermoMPNN
## 1815	-14.33546886	0.046170711	0 2432	ThermoMPNN
## 1816	-19.14455261	-0.116001141	0 2428	ThermoMPNN
## 1817	-21.06043510	0.332911304	0 2443	ThermoMPNN
## 1818	-19.40548019	-0.624398657	0 2451	ThermoMPNN
## 1819	-20.60336342	0.014121685	0 2442	ThermoMPNN
## 1820	-17.23811226	-0.013947432	0 2446	ThermoMPNN
## 1821	-14.74432888	-0.011567739	0 2455	ThermoMPNN
## 1822	-18.17353439	-0.126521015	0 2456	ThermoMPNN
## 1823	-17.37025185	-0.017653484	0 2445	ThermoMPNN
## 1824	-15.76734409	-0.438289467	0 2450	ThermoMPNN
## 1825	-19.46564636	-0.313656395	0 2453	ThermoMPNN
## 1826	-14.52961597	-0.284143478	0 2447	ThermoMPNN
## 1827	-14.65457592	0.067281358	0 2441	ThermoMPNN
## 1828	-18.21349239	-0.044912223	0 2454	ThermoMPNN
## 1829	-17.70361900	0.076788247	0 2440	ThermoMPNN
## 1830	-11.61321182	-0.157859902	0 2449	ThermoMPNN
## 1831	-21.32037277	-0.353327445	0 2448	ThermoMPNN
## 1832	-12.82204323	-0.488389654	0 2459	ThermoMPNN
## 1833	-14.33516521	-0.123940449	0 2458	ThermoMPNN
## 1834	-19.48898201	-0.288959063	0 2452	ThermoMPNN
## 1835	-14.23094330	-0.069652977	0 2457	ThermoMPNN
## 1836	-14.36176662	0.172678793	0 2473	ThermoMPNN
## 1837	-15.46289520	-0.291357760	0 2467	ThermoMPNN
## 1838	-16.01742592	-0.197894962	0 2464	ThermoMPNN
## 1839	-10.62846222	0.345738707	0 2465	ThermoMPNN
## 1840	-11.56713142	0.150691687	0 2460	ThermoMPNN
## 1841	-14.74565697	0.256372106	0 2461	ThermoMPNN

## 1842	-18.94358482	-0.232341066	0 2472	ThermoMPNN
## 1843	-15.87456112	0.445762263	0 2469	ThermoMPNN
## 1844	-14.57989674	0.222124729	0 2468	ThermoMPNN
## 1845	-10.19830742	0.122582022	0 2463	ThermoMPNN
## 1846	-15.38377934	0.108358136	0 2474	ThermoMPNN
## 1847	-13.42418747	-0.050779706	0 2477	ThermoMPNN
## 1848	-11.19886990	0.224380939	0 2475	ThermoMPNN
## 1849	-16.38964176	0.048198996	0 2470	ThermoMPNN
## 1850	-18.56979904	-0.169485010	0 2478	ThermoMPNN
## 1851	-13.03097458	-0.008089124	0 2476	ThermoMPNN
## 1852	-15.51686535	0.019909575	0 2480	ThermoMPNN
## 1853	-10.45186253	0.110700212	0 2481	ThermoMPNN
## 1854	-15.53043652	0.031655556	0 2482	ThermoMPNN
## 1855	-17.17155895	-0.189466958	0 2483	ThermoMPNN
## 1856	-5.89940510	0.358656215	0 2484	ThermoMPNN
## 1857	-15.74741020	1.135419838	1 2485	ThermoMPNN
## 1858	-5.46369219	0.851091922	1 2486	ThermoMPNN
## 1859	-16.21085300	0.272072970	0 2487	ThermoMPNN
## 1860	-16.56882877	0.410900478	0 2488	ThermoMPNN
## 1861	-13.41364594	0.122658659	0 2489	ThermoMPNN
## 1862	-16.11389618	-0.245120868	0 2490	ThermoMPNN
## 1863	-12.45038166	-0.019226913	0 2491	ThermoMPNN
## 1864	-16.95340614	-0.031720248	0 2492	ThermoMPNN
## 1865	-14.33091393	0.009047403	0 2493	ThermoMPNN
## 1866	-12.91210384	0.193605430	0 2494	ThermoMPNN
## 1867	-11.67094021	0.148138630	0 2495	ThermoMPNN
## 1868	-16.06972599	-0.007147707	0 2496	ThermoMPNN
## 1869	-15.43734150	0.112713283	0 2497	ThermoMPNN
## 1870	-14.28602295	-0.226485850	0 2498	ThermoMPNN
## 1871	-18.00723724	-0.293844645	0 2508	ThermoMPNN
## 1872	-17.02713623	-0.212811674	0 2505	ThermoMPNN
## 1873	-14.12724457	-0.236679494	0 2501	ThermoMPNN
## 1874	-13.84666805	0.082860984	0 2500	ThermoMPNN
## 1875	-18.51618805	0.052261103	0 2506	ThermoMPNN
## 1876	-9.12243271	0.065449952	0 2510	ThermoMPNN
## 1877	-18.19503689	0.116801320	0 2503	ThermoMPNN
## 1878	-18.85327797	-0.299794740	0 2502	ThermoMPNN
## 1879	-8.00700369	0.309259927	0 2509	ThermoMPNN
## 1880	-12.62940350	0.390742507	0 2504	ThermoMPNN
## 1881	-8.37888603	1.000132685	1 2517	ThermoMPNN
## 1882	-16.69473915	0.179217464	0 2519	ThermoMPNN
## 1883	-18.99855137	-0.319904888	0 2518	ThermoMPNN
## 1884	-15.96883736	-0.391138846	0 2511	ThermoMPNN
## 1885	-17.20094147	-0.196717363	0 2512	ThermoMPNN
## 1886	-10.81147852	0.192148492	0 2516	ThermoMPNN
## 1887	-17.38561993	-0.506479871	0 2513	ThermoMPNN
## 1888	-13.46817112	-0.215234161	0 2515	ThermoMPNN
## 1889	-18.43546867	0.254675569	0 2514	ThermoMPNN
## 1890	-1.14027872	0.807409068	1 2520	ThermoMPNN
## 1891	-9.37970209	0.682203979	1 2521	ThermoMPNN
## 1892	-12.83845558	-0.198540848	0 2522	ThermoMPNN
## 1893	-12.02647934	0.106401760	0 2523	ThermoMPNN
## 1894	-12.24850998	0.551672297	0 2524	ThermoMPNN
## 1895	-7.89961824	1.853945734	1 2525	ThermoMPNN

## 1896	-14.64668694	-0.006069709	0 2526	ThermoMPNN
## 1897	-11.25081005	0.484250980	0 2527	ThermoMPNN
## 1898	-14.37835350	0.334578650	0 2528	ThermoMPNN
## 1899	-12.52939625	-0.093947342	0 2529	ThermoMPNN
## 1900	-12.70885544	-0.470178979	0 2531	ThermoMPNN
## 1901	-12.32689915	0.109423812	0 2532	ThermoMPNN
## 1902	-13.47565231	0.084621322	0 2534	ThermoMPNN
## 1903	-7.22536135	-0.115428277	0 2536	ThermoMPNN
## 1904	-6.68688545	1.598159470	1 2537	ThermoMPNN
## 1905	-14.40534077	0.113358310	0 2538	ThermoMPNN
## 1906	-10.66177597	1.837600179	1 2550	ThermoMPNN
## 1907	-13.53815594	1.430631562	1 2559	ThermoMPNN
## 1908	-9.73827658	0.628736957	1 2549	ThermoMPNN
## 1909	-8.24329290	1.070482115	1 2548	ThermoMPNN
## 1910	-7.90758138	0.413413065	0 2545	ThermoMPNN
## 1911	-9.80520496	0.860355089	1 2546	ThermoMPNN
## 1912	-14.59258690	0.504254487	0 2558	ThermoMPNN
## 1913	-13.43941345	1.087901857	1 2544	ThermoMPNN
## 1914	-7.83124628	0.679150279	1 2540	ThermoMPNN
## 1915	-9.72595201	0.734624878	1 2551	ThermoMPNN
## 1916	-11.45752316	0.469915725	0 2547	ThermoMPNN
## 1917	-9.15531445	0.605038276	1 2557	ThermoMPNN
## 1918	-11.53080912	1.679847186	1 2541	ThermoMPNN
## 1919	-8.58795466	1.154718891	1 2555	ThermoMPNN
## 1920	-9.84336724	0.475161500	0 2554	ThermoMPNN
## 1921	-15.52238274	-0.063976783	0 2552	ThermoMPNN
## 1922	-9.25029912	0.356887138	0 2556	ThermoMPNN
## 1923	-5.40793667	-0.116279786	0 2553	ThermoMPNN
## 1924	-12.70762901	0.101409441	0 2576	ThermoMPNN
## 1925	-10.08413343	0.834052520	1 2560	ThermoMPNN
## 1926	-13.03406029	-0.321121793	0 2577	ThermoMPNN
## 1927	-13.93782444	0.598613928	1 2568	ThermoMPNN
## 1928	-14.34467754	-0.135136699	0 2569	ThermoMPNN
## 1929	-14.82736073	0.009346123	0 2567	ThermoMPNN
## 1930	-8.30782976	0.142465150	0 2575	ThermoMPNN
## 1931	-12.62792168	-0.060772646	0 2571	ThermoMPNN
## 1932	-17.79190407	-0.144320993	0 2572	ThermoMPNN
## 1933	-15.38090553	0.464309529	0 2570	ThermoMPNN
## 1934	-16.75754375	-0.276714194	0 2562	ThermoMPNN
## 1935	-14.02024879	0.104882354	0 2578	ThermoMPNN
## 1936	-14.86999168	0.082514627	0 2573	ThermoMPNN
## 1937	-15.06593704	-0.622496479	0 2563	ThermoMPNN
## 1938	-14.52343197	0.324116813	0 2566	ThermoMPNN
## 1939	-10.81231670	0.166420859	0 2574	ThermoMPNN
## 1940	-11.45550089	0.760833313	1 2565	ThermoMPNN
## 1941	-17.05097885	-0.063292768	0 2583	ThermoMPNN
## 1942	-11.24959164	0.399132620	0 2584	ThermoMPNN
## 1943	-9.12828217	-0.384644547	0 2596	ThermoMPNN
## 1944	-15.94380207	0.159152494	0 2585	ThermoMPNN
## 1945	-14.47844830	-0.228097036	0 2581	ThermoMPNN
## 1946	-16.35080986	-0.229041976	0 2594	ThermoMPNN
## 1947	-13.19323807	-0.112425441	0 2595	ThermoMPNN
## 1948	-16.65652084	-0.214153030	0 2588	ThermoMPNN
## 1949	-6.03165140	0.288645063	0 2597	ThermoMPNN

## 1950	-17.40981960	0.251077253	0 2598	ThermoMPNN
## 1951	-17.68529949	-0.381006968	0 2586	ThermoMPNN
## 1952	-16.69558887	-0.446184459	0 2599	ThermoMPNN
## 1953	-5.05568657	0.429639445	0 2589	ThermoMPNN
## 1954	-16.67513924	-0.267583715	0 2593	ThermoMPNN
## 1955	-15.89984818	-0.179841820	0 2591	ThermoMPNN
## 1956	-11.32796288	0.102379088	0 2580	ThermoMPNN
## 1957	-15.17051964	-0.148605424	0 2592	ThermoMPNN
## 1958	-6.50042677	-0.023250417	0 2600	ThermoMPNN
## 1959	-9.62979164	0.682731993	1 2601	ThermoMPNN
## 1960	-12.51886578	0.326621003	0 2602	ThermoMPNN
## 1961	-11.37466469	0.269443520	0 2603	ThermoMPNN
## 1962	-11.19329185	0.352193763	0 2604	ThermoMPNN
## 1963	-8.50340405	1.911713135	1 2605	ThermoMPNN
## 1964	-11.51186543	-0.158995866	0 2606	ThermoMPNN
## 1965	-12.08821640	0.410260053	0 2607	ThermoMPNN
## 1966	-11.65855236	0.087631147	0 2608	ThermoMPNN
## 1967	-11.09280262	0.046581826	0 2609	ThermoMPNN
## 1968	-12.39738693	0.795312885	1 2610	ThermoMPNN
## 1969	-10.36907425	0.200296834	0 2611	ThermoMPNN
## 1970	-12.72424488	-0.173256461	0 2612	ThermoMPNN
## 1971	-10.02365599	-0.123262933	0 2613	ThermoMPNN
## 1972	-10.83258352	0.848116827	1 2614	ThermoMPNN
## 1973	-8.52774611	-0.017682374	0 2616	ThermoMPNN
## 1974	-11.04760494	-0.002257892	0 2617	ThermoMPNN
## 1975	-12.89878960	0.249478694	0 2618	ThermoMPNN
## 1976	-11.98297653	0.389206314	0 2619	ThermoMPNN
## 1977	-8.05983896	0.526466846	0 2635	ThermoMPNN
## 1978	-9.14663458	0.148997655	0 2636	ThermoMPNN
## 1979	-10.17137280	0.020226854	0 2637	ThermoMPNN
## 1980	-11.28199902	0.791599007	1 2630	ThermoMPNN
## 1981	-7.22061596	0.079329178	0 2625	ThermoMPNN
## 1982	-11.89257479	0.005808150	0 2624	ThermoMPNN
## 1983	-10.21408367	0.546121778	0 2634	ThermoMPNN
## 1984	-15.91429119	-0.235587609	0 2632	ThermoMPNN
## 1985	-10.77794113	0.080361697	0 2627	ThermoMPNN
## 1986	-6.21854181	1.070488937	1 2623	ThermoMPNN
## 1987	-11.61344910	0.028609744	0 2621	ThermoMPNN
## 1988	-13.75872116	0.016846853	0 2638	ThermoMPNN
## 1989	-10.14089556	0.699796717	1 2629	ThermoMPNN
## 1990	-11.14657049	0.759558524	1 2639	ThermoMPNN
## 1991	-9.07092400	-0.096474540	0 2633	ThermoMPNN
## 1992	-6.33114309	0.718010530	1 2631	ThermoMPNN
## 1993	-9.28771667	0.607995017	1 2626	ThermoMPNN
## 1994	-9.09013243	0.687636466	1 2620	ThermoMPNN
## 1995	-8.30159321	1.187979421	1 2628	ThermoMPNN
## 1996	-19.28750534	0.172055900	0 2648	ThermoMPNN
## 1997	-18.46862831	-0.232543731	0 2653	ThermoMPNN
## 1998	-18.49143715	-0.135041863	0 2643	ThermoMPNN
## 1999	-19.50503082	-0.519192196	0 2642	ThermoMPNN
## 2000	-15.17887383	-0.235226405	0 2641	ThermoMPNN
## 2001	-15.15116425	-0.168189234	0 2647	ThermoMPNN
## 2002	-21.33016281	-0.022310136	0 2652	ThermoMPNN
## 2003	-16.34941559	0.526940529	0 2650	ThermoMPNN

## 2004	-18.54229202	0.001685789	0 2654	ThermoMPNN
## 2005	-15.82956982	0.205677999	0 2646	ThermoMPNN
## 2006	-18.75049381	-0.035530990	0 2645	ThermoMPNN
## 2007	-15.18675003	-0.163217781	0 2657	ThermoMPNN
## 2008	-17.16931057	-0.537960564	0 2640	ThermoMPNN
## 2009	-13.27329445	0.193255460	0 2649	ThermoMPNN
## 2010	-18.05015450	-0.256761196	0 2651	ThermoMPNN
## 2011	-11.90050030	0.253004402	0 2659	ThermoMPNN
## 2012	-17.07243156	0.147831850	0 2656	ThermoMPNN
## 2013	-17.60919323	-0.114700594	0 2658	ThermoMPNN
## 2014	-15.86171684	0.408432441	0 2655	ThermoMPNN
## 2015	-9.46364269	0.386572069	0 2667	ThermoMPNN
## 2016	-16.85030022	-0.241227764	0 2671	ThermoMPNN
## 2017	-16.32583942	-0.128576881	0 2665	ThermoMPNN
## 2018	-15.17212868	0.043839342	0 2666	ThermoMPNN
## 2019	-13.95801754	-0.087761751	0 2675	ThermoMPNN
## 2020	-15.14534340	0.179694132	0 2661	ThermoMPNN
## 2021	-15.89043064	-0.252651281	0 2679	ThermoMPNN
## 2022	-16.36579418	-0.405961770	0 2678	ThermoMPNN
## 2023	-14.25002537	-0.094732855	0 2674	ThermoMPNN
## 2024	-9.44397945	0.814913325	1 2677	ThermoMPNN
## 2025	-15.54718647	-0.093259261	0 2668	ThermoMPNN
## 2026	-13.38531952	-0.212584889	0 2673	ThermoMPNN
## 2027	-12.95132389	0.493842000	0 2660	ThermoMPNN
## 2028	-14.69898396	-0.186370256	0 2672	ThermoMPNN
## 2029	-16.64059944	-0.033571903	0 2663	ThermoMPNN
## 2030	-12.84102211	0.245769500	0 2676	ThermoMPNN
## 2031	-18.46070824	0.021122643	0 2662	ThermoMPNN
## 2032	-13.67107449	0.744040672	1 2698	ThermoMPNN
## 2033	-8.86642780	0.776534008	1 2697	ThermoMPNN
## 2034	-10.81092663	-0.005974237	0 2687	ThermoMPNN
## 2035	-10.81943245	1.102167629	1 2689	ThermoMPNN
## 2036	-9.27917843	0.480476629	0 2695	ThermoMPNN
## 2037	-11.50031490	0.632153718	1 2690	ThermoMPNN
## 2038	-9.20702381	0.264499493	0 2685	ThermoMPNN
## 2039	-11.65966034	0.201894945	0 2684	ThermoMPNN
## 2040	-9.09424095	0.665958408	1 2696	ThermoMPNN
## 2041	-8.68706093	0.219243108	0 2680	ThermoMPNN
## 2042	-8.95346336	0.754079564	1 2686	ThermoMPNN
## 2043	-5.56012506	0.557490005	0 2683	ThermoMPNN
## 2044	-9.77104969	0.767347058	1 2693	ThermoMPNN
## 2045	-11.80557537	1.173452883	1 2694	ThermoMPNN
## 2046	-7.69897623	0.879882219	1 2691	ThermoMPNN
## 2047	-16.56229401	0.107634207	0 2692	ThermoMPNN
## 2048	-11.95997944	0.880030192	1 2681	ThermoMPNN
## 2049	-10.85686102	0.513095605	0 2717	ThermoMPNN
## 2050	-8.13081827	1.187513566	1 2706	ThermoMPNN
## 2051	-9.36781559	-0.095457844	0 2719	ThermoMPNN
## 2052	-10.26689901	0.283593393	0 2705	ThermoMPNN
## 2053	-8.12503529	0.680498790	1 2715	ThermoMPNN
## 2054	-7.75863361	0.898626162	1 2716	ThermoMPNN
## 2055	-10.04925919	0.580153732	1 2704	ThermoMPNN
## 2056	-10.63923836	0.549946180	0 2701	ThermoMPNN
## 2057	-13.20424442	0.333945936	0 2718	ThermoMPNN

## 2058	-9.65729141	0.349211870	0 2700	ThermoMPNN
## 2059	-9.54975090	1.205779659	1 2710	ThermoMPNN
## 2060	-6.91254663	0.828404097	1 2714	ThermoMPNN
## 2061	-10.10366278	1.484592736	1 2702	ThermoMPNN
## 2062	-9.85431900	0.472075017	0 2709	ThermoMPNN
## 2063	-9.15747099	0.972605470	1 2703	ThermoMPNN
## 2064	-9.91283178	0.894156823	1 2707	ThermoMPNN
## 2065	-8.23391485	0.988512488	1 2713	ThermoMPNN
## 2066	-15.22330933	0.025676315	0 2712	ThermoMPNN
## 2067	-10.00149908	0.652158018	1 2724	ThermoMPNN
## 2068	-14.12228355	0.554246346	0 2732	ThermoMPNN
## 2069	-6.71529603	1.314585094	1 2733	ThermoMPNN
## 2070	-13.54273033	1.115953632	1 2725	ThermoMPNN
## 2071	-10.15321732	0.811069852	1 2723	ThermoMPNN
## 2072	-13.01691246	0.937863449	1 2736	ThermoMPNN
## 2073	-11.74280653	2.079843809	1 2727	ThermoMPNN
## 2074	-10.27091818	0.786431856	1 2734	ThermoMPNN
## 2075	-11.74644756	1.042103428	1 2735	ThermoMPNN
## 2076	-8.50086946	0.294708393	0 2731	ThermoMPNN
## 2077	-13.56254101	0.574928412	1 2720	ThermoMPNN
## 2078	-12.10933599	1.382090000	1 2737	ThermoMPNN
## 2079	-13.08254318	-0.012597213	0 2722	ThermoMPNN
## 2080	-8.18661318	2.086013846	1 2730	ThermoMPNN
## 2081	-12.05649471	0.541552512	0 2738	ThermoMPNN
## 2082	-12.55398865	1.430441091	1 2721	ThermoMPNN
## 2083	-10.55648851	0.499950933	0 2728	ThermoMPNN
## 2084	-8.97244434	0.530795896	0 2739	ThermoMPNN
## 2085	-7.90644751	1.414559903	1 2729	ThermoMPNN
## 2086	-9.32980347	0.912173380	1 2749	ThermoMPNN
## 2087	-10.64140320	0.818567695	1 2750	ThermoMPNN
## 2088	-12.36771431	0.066662388	0 2752	ThermoMPNN
## 2089	-7.79172964	0.839187203	1 2754	ThermoMPNN
## 2090	-9.65470171	0.712975680	1 2740	ThermoMPNN
## 2091	-6.23585737	1.614078758	1 2751	ThermoMPNN
## 2092	-5.21711617	-0.077711682	0 2743	ThermoMPNN
## 2093	-6.92461653	0.658101900	1 2748	ThermoMPNN
## 2094	-12.40021839	0.868310928	1 2758	ThermoMPNN
## 2095	-9.71672764	-0.045002707	0 2741	ThermoMPNN
## 2096	-12.13167458	0.796362103	1 2747	ThermoMPNN
## 2097	-11.14376841	1.130428048	1 2756	ThermoMPNN
## 2098	-11.14189081	0.405705696	0 2744	ThermoMPNN
## 2099	-9.98213758	0.224061395	0 2759	ThermoMPNN
## 2100	-8.49631462	1.096822828	1 2755	ThermoMPNN
## 2101	-5.05851784	1.355290212	1 2746	ThermoMPNN
## 2102	-10.88081684	1.101783512	1 2757	ThermoMPNN
## 2103	-6.70881481	0.431893946	0 2745	ThermoMPNN
## 2104	-13.50154591	0.021970057	0 2761	ThermoMPNN
## 2105	-10.65927715	0.126733507	0 2760	ThermoMPNN
## 2106	-12.62553177	1.025513574	1 2774	ThermoMPNN
## 2107	-11.91671524	0.321412243	0 2775	ThermoMPNN
## 2108	-6.74443483	0.618064562	1 2777	ThermoMPNN
## 2109	-14.14738445	0.224526806	0 2778	ThermoMPNN
## 2110	-6.19469194	0.502264051	0 2767	ThermoMPNN
## 2111	-14.46701050	0.330763432	0 2762	ThermoMPNN

## 2112	-9.51616764	1.433231863	1 2776	ThermoMPNN
## 2113	-12.11750793	0.753521796	1 2773	ThermoMPNN
## 2114	-10.23801527	0.283071084	0 2764	ThermoMPNN
## 2115	-5.88080244	0.495015279	0 2769	ThermoMPNN
## 2116	-13.00423546	-0.056307572	0 2763	ThermoMPNN
## 2117	-13.26145191	0.357026610	0 2771	ThermoMPNN
## 2118	-13.48072758	0.457345952	0 2772	ThermoMPNN
## 2119	-13.06352367	0.254907998	0 2765	ThermoMPNN
## 2120	-13.21741982	1.148474713	1 2766	ThermoMPNN
## 2121	-13.21527596	0.819580696	1 2779	ThermoMPNN
## 2122	-11.26955109	0.194056136	0 2787	ThermoMPNN
## 2123	-9.84957485	-0.164439864	0 2786	ThermoMPNN
## 2124	-8.97548122	0.375561416	0 2796	ThermoMPNN
## 2125	-11.79431610	0.239800272	0 2785	ThermoMPNN
## 2126	-11.38924637	0.114077194	0 2780	ThermoMPNN
## 2127	-11.38562279	0.238472352	0 2789	ThermoMPNN
## 2128	-11.75099640	0.078286121	0 2797	ThermoMPNN
## 2129	-14.08346958	0.081714444	0 2798	ThermoMPNN
## 2130	-9.98337030	0.445336130	0 2790	ThermoMPNN
## 2131	-12.88798409	0.148343587	0 2792	ThermoMPNN
## 2132	-12.23668499	-0.170319293	0 2799	ThermoMPNN
## 2133	-11.71000977	0.010920513	0 2781	ThermoMPNN
## 2134	-12.25099487	0.169523198	0 2782	ThermoMPNN
## 2135	-8.57786636	-0.075843587	0 2791	ThermoMPNN
## 2136	-13.35096493	-0.003339938	0 2784	ThermoMPNN
## 2137	-9.23485699	0.077210861	0 2793	ThermoMPNN
## 2138	-10.82074642	1.793691865	1 2783	ThermoMPNN
## 2139	-9.74598875	0.443753139	0 2795	ThermoMPNN
## 2140	-6.91523361	0.736756995	1 2794	ThermoMPNN
## 2141	-10.69849377	0.439373084	0 2803	ThermoMPNN
## 2142	-12.59684467	0.139730968	0 2812	ThermoMPNN
## 2143	-13.65334053	0.138590575	0 2807	ThermoMPNN
## 2144	-13.09867516	0.089278679	0 2810	ThermoMPNN
## 2145	-11.17351952	0.232569994	0 2804	ThermoMPNN
## 2146	-9.06665077	0.502468748	0 2802	ThermoMPNN
## 2147	-9.28881617	0.943733292	1 2813	ThermoMPNN
## 2148	-11.69277859	-0.167054836	0 2809	ThermoMPNN
## 2149	-11.28989296	0.164807868	0 2801	ThermoMPNN
## 2150	-9.63794289	0.264516108	0 2814	ThermoMPNN
## 2151	-7.30111313	0.293329295	0 2811	ThermoMPNN
## 2152	-9.30718088	1.178861684	1 2805	ThermoMPNN
## 2153	-13.57508373	1.731663158	1 2818	ThermoMPNN
## 2154	-12.22677269	-0.010463053	0 2800	ThermoMPNN
## 2155	-10.94796839	0.254530654	0 2808	ThermoMPNN
## 2156	-8.13823109	0.541348749	0 2819	ThermoMPNN
## 2157	-13.06006947	0.528714654	0 2817	ThermoMPNN
## 2158	-9.86417322	0.279791821	0 2815	ThermoMPNN
## 2159	-11.42515945	0.410085139	0 2816	ThermoMPNN
## 2160	-9.07151051	0.290465908	0 2836	ThermoMPNN
## 2161	-13.65899868	-0.178440336	0 2838	ThermoMPNN
## 2162	-14.37348728	0.805769012	1 2839	ThermoMPNN
## 2163	-12.08213787	0.508823532	0 2837	ThermoMPNN
## 2164	-10.45420742	0.798460743	1 2831	ThermoMPNN
## 2165	-11.05299454	0.292195219	0 2829	ThermoMPNN

## 2166	-10.75019169	0.380243097	0 2835	ThermoMPNN
## 2167	-13.51870289	-0.249719495	0 2832	ThermoMPNN
## 2168	-11.35040398	0.269678349	0 2820	ThermoMPNN
## 2169	-6.86432581	1.458471284	1 2834	ThermoMPNN
## 2170	-12.83005924	0.448335346	0 2821	ThermoMPNN
## 2171	-8.24207630	0.492304931	0 2823	ThermoMPNN
## 2172	-8.40015373	0.561290272	0 2833	ThermoMPNN
## 2173	-12.36436405	0.111709059	0 2827	ThermoMPNN
## 2174	-11.93326855	0.497024038	0 2822	ThermoMPNN
## 2175	-11.61137352	0.432640303	0 2825	ThermoMPNN
## 2176	-10.80421219	0.616948787	1 2826	ThermoMPNN
## 2177	-14.71917210	0.282605524	0 2824	ThermoMPNN
## 2178	-11.78651142	0.069227115	0 2852	ThermoMPNN
## 2179	-9.00933008	0.707462180	1 2851	ThermoMPNN
## 2180	-13.42992859	0.354650060	0 2844	ThermoMPNN
## 2181	-10.92932796	0.023775656	0 2840	ThermoMPNN
## 2182	-9.81517372	0.185137178	0 2853	ThermoMPNN
## 2183	-13.56845360	0.668940456	1 2859	ThermoMPNN
## 2184	-13.24371033	0.159389513	0 2842	ThermoMPNN
## 2185	-12.43388062	0.271928654	0 2845	ThermoMPNN
## 2186	-14.23206863	0.778342908	1 2858	ThermoMPNN
## 2187	-12.05513763	0.439230689	0 2841	ThermoMPNN
## 2188	-10.88221321	-0.039452975	0 2846	ThermoMPNN
## 2189	-11.40344143	0.313488303	0 2843	ThermoMPNN
## 2190	-8.20244846	0.516668560	0 2856	ThermoMPNN
## 2191	-10.11825027	-0.076421609	0 2850	ThermoMPNN
## 2192	-10.63354378	0.732182368	1 2857	ThermoMPNN
## 2193	-6.60172291	0.686648837	1 2854	ThermoMPNN
## 2194	-9.55410099	0.288098623	0 2855	ThermoMPNN
## 2195	-11.18453255	-0.192876052	0 2849	ThermoMPNN
## 2196	-10.10300903	0.441146150	0 2847	ThermoMPNN
## 2197	-10.26530685	0.750079721	1 2870	ThermoMPNN
## 2198	-14.18370247	-0.116141392	0 2876	ThermoMPNN
## 2199	-10.78548222	0.269952602	0 2867	ThermoMPNN
## 2200	-14.84887714	-0.003058988	0 2868	ThermoMPNN
## 2201	-16.55185699	0.079492078	0 2865	ThermoMPNN
## 2202	-14.50737152	1.024391764	1 2875	ThermoMPNN
## 2203	-16.79420452	0.637029528	1 2871	ThermoMPNN
## 2204	-15.28172226	0.222826950	0 2860	ThermoMPNN
## 2205	-12.38339252	1.248842922	1 2874	ThermoMPNN
## 2206	-18.44206581	-0.107028753	0 2862	ThermoMPNN
## 2207	-12.41736660	0.663171387	1 2872	ThermoMPNN
## 2208	-13.49345665	0.906114090	1 2866	ThermoMPNN
## 2209	-13.67680035	0.289463484	0 2878	ThermoMPNN
## 2210	-13.87842655	0.698712454	1 2879	ThermoMPNN
## 2211	-11.29341183	0.227368387	0 2877	ThermoMPNN
## 2212	-13.05091648	0.089968663	0 2873	ThermoMPNN
## 2213	-17.30803280	0.030515294	0 2863	ThermoMPNN
## 2214	-10.20002756	0.427925199	0 2864	ThermoMPNN
## 2215	-11.38542156	1.177548393	1 2889	ThermoMPNN
## 2216	-15.84690685	2.213596493	1 2890	ThermoMPNN
## 2217	-12.62906227	2.398564801	1 2893	ThermoMPNN
## 2218	-13.56310444	3.073866884	1 2894	ThermoMPNN
## 2219	-11.27868805	1.638179714	1 2880	ThermoMPNN

## 2220	-14.53178539	1.385449736	1 2891	ThermoMPNN
## 2221	-12.27009773	1.365883895	1 2886	ThermoMPNN
## 2222	-15.62557487	0.950698431	1 2887	ThermoMPNN
## 2223	-16.90420265	0.285074967	0 2898	ThermoMPNN
## 2224	-13.31814756	2.195697103	1 2899	ThermoMPNN
## 2225	-13.47742252	1.372727703	1 2881	ThermoMPNN
## 2226	-15.39063206	0.964107992	1 2882	ThermoMPNN
## 2227	-15.04766769	0.983610945	1 2883	ThermoMPNN
## 2228	-13.72465973	1.123657666	1 2884	ThermoMPNN
## 2229	-14.71019611	2.176386953	1 2885	ThermoMPNN
## 2230	-13.38996925	1.514255001	1 2896	ThermoMPNN
## 2231	-14.81004505	1.722659819	1 2897	ThermoMPNN
## 2232	-10.67508278	2.332323346	1 2895	ThermoMPNN
## 2233	-18.87407265	-0.660693243	0 2902	ThermoMPNN
## 2234	-17.90900803	-0.016563867	0 2903	ThermoMPNN
## 2235	-13.30196342	-0.039292889	0 2912	ThermoMPNN
## 2236	-15.93415661	-0.225278120	0 2901	ThermoMPNN
## 2237	-16.61111698	0.016185723	0 2908	ThermoMPNN
## 2238	-14.42985058	0.131587119	0 2914	ThermoMPNN
## 2239	-14.10344353	-0.403098220	0 2913	ThermoMPNN
## 2240	-14.21699772	-0.006922944	0 2906	ThermoMPNN
## 2241	-17.77650414	-0.015021271	0 2911	ThermoMPNN
## 2242	-15.84492455	-0.029662696	0 2918	ThermoMPNN
## 2243	-17.75273857	-0.132391898	0 2905	ThermoMPNN
## 2244	-15.35909328	-0.146616663	0 2915	ThermoMPNN
## 2245	-11.38091412	-0.253538304	0 2907	ThermoMPNN
## 2246	-11.55375385	-0.024591858	0 2917	ThermoMPNN
## 2247	-16.08905525	-0.181071783	0 2919	ThermoMPNN
## 2248	-15.04550800	0.249271630	0 2916	ThermoMPNN
## 2249	-14.63986244	0.295594357	0 2900	ThermoMPNN
## 2250	-19.10026703	-0.051667402	0 2927	ThermoMPNN
## 2251	-18.75636063	0.235192814	0 2939	ThermoMPNN
## 2252	-15.51638889	-0.219141196	0 2923	ThermoMPNN
## 2253	-19.40389824	-0.161946790	0 2924	ThermoMPNN
## 2254	-18.52946014	-0.135468310	0 2926	ThermoMPNN
## 2255	-18.06712303	-0.067489059	0 2928	ThermoMPNN
## 2256	-17.35324821	-0.181440880	0 2938	ThermoMPNN
## 2257	-11.81479454	-0.028750566	0 2920	ThermoMPNN
## 2258	-14.98465900	0.274250598	0 2922	ThermoMPNN
## 2259	-15.88733959	0.050640074	0 2937	ThermoMPNN
## 2260	-12.68863811	-0.016166570	0 2935	ThermoMPNN
## 2261	-16.36076298	0.533956853	0 2936	ThermoMPNN
## 2262	-13.49064846	-0.128751732	0 2934	ThermoMPNN
## 2263	-18.80728149	0.267120141	0 2933	ThermoMPNN
## 2264	-16.64515667	-0.551353658	0 2931	ThermoMPNN
## 2265	-18.57270927	0.794130915	1 2929	ThermoMPNN
## 2266	-19.19677582	0.052375149	0 2930	ThermoMPNN
## 2267	-19.06712799	0.318987701	0 2932	ThermoMPNN
## 2268	-14.78144550	-0.060748090	0 2947	ThermoMPNN
## 2269	-20.60898819	-0.182896598	0 2945	ThermoMPNN
## 2270	-15.87435741	1.393248835	1 2950	ThermoMPNN
## 2271	-19.44255180	-0.188216183	0 2953	ThermoMPNN
## 2272	-22.23505211	0.096995126	0 2943	ThermoMPNN
## 2273	-17.07843456	0.004977573	0 2946	ThermoMPNN

## 2274	-21.54891205	-0.046445555	0 2948	ThermoMPNN
## 2275	-20.17547684	-0.012182925	0 2954	ThermoMPNN
## 2276	-18.70992126	-0.200569949	0 2952	ThermoMPNN
## 2277	-21.86149445	-0.243834615	0 2942	ThermoMPNN
## 2278	-17.93688736	-0.273655917	0 2958	ThermoMPNN
## 2279	-19.87711563	-0.313045799	0 2951	ThermoMPNN
## 2280	-16.97781448	-0.010554985	0 2955	ThermoMPNN
## 2281	-15.46417999	-0.072626634	0 2941	ThermoMPNN
## 2282	-19.38002357	0.060379970	0 2956	ThermoMPNN
## 2283	-11.59298744	0.289083230	0 2949	ThermoMPNN
## 2284	-15.39236355	0.486274967	0 2957	ThermoMPNN
## 2285	-18.77952995	-0.012572291	0 2940	ThermoMPNN
## 2286	-11.21937313	1.540441590	1 2960	ThermoMPNN
## 2287	-14.68326931	2.983151878	1 2961	ThermoMPNN
## 2288	-17.05179996	0.083015133	0 2962	ThermoMPNN
## 2289	-19.38543167	0.306385287	0 2963	ThermoMPNN
## 2290	-19.12379761	0.095783979	0 2964	ThermoMPNN
## 2291	-16.16553078	0.818024824	1 2965	ThermoMPNN
## 2292	-19.33922157	-0.053277914	0 2966	ThermoMPNN
## 2293	-14.00552254	-0.123840299	0 2967	ThermoMPNN
## 2294	-17.90669937	-0.158865350	0 2968	ThermoMPNN
## 2295	-17.50310173	0.095406947	0 2969	ThermoMPNN
## 2296	-15.34845333	-0.333327362	0 2970	ThermoMPNN
## 2297	-15.29282684	0.038561633	0 2971	ThermoMPNN
## 2298	-15.08329983	0.131552611	0 2972	ThermoMPNN
## 2299	-20.15575066	0.322509817	0 2973	ThermoMPNN
## 2300	-17.49706268	0.038071698	0 2974	ThermoMPNN
## 2301	-12.33109455	0.247863759	0 2975	ThermoMPNN
## 2302	-13.28709660	-0.055154394	0 2977	ThermoMPNN
## 2303	-21.63718071	0.130045646	0 2978	ThermoMPNN
## 2304	-19.37269211	0.005363449	0 2979	ThermoMPNN
## 2305	-19.90862923	-0.042931000	0 2991	ThermoMPNN
## 2306	-15.68779411	0.093091947	0 2995	ThermoMPNN
## 2307	-17.18176842	0.118613815	0 2986	ThermoMPNN
## 2308	-20.37230110	0.244100694	0 2993	ThermoMPNN
## 2309	-15.00882721	0.331220344	0 2987	ThermoMPNN
## 2310	-18.98880920	0.059796887	0 2992	ThermoMPNN
## 2311	-14.97710648	0.073615230	0 2997	ThermoMPNN
## 2312	-16.46146851	-0.107390647	0 2998	ThermoMPNN
## 2313	-17.28538837	0.000784664	0 2990	ThermoMPNN
## 2314	-21.77017403	0.007168001	0 2988	ThermoMPNN
## 2315	-12.86125813	0.253330804	0 2989	ThermoMPNN
## 2316	-19.98786354	-0.032315776	0 2985	ThermoMPNN
## 2317	-19.56904030	-0.052512560	0 2994	ThermoMPNN
## 2318	-20.49093056	0.089096647	0 2982	ThermoMPNN
## 2319	-19.23185921	-0.036935034	0 2996	ThermoMPNN
## 2320	-21.80298882	-0.048122831	0 2983	ThermoMPNN
## 2321	-14.88806725	-0.092066927	0 2981	ThermoMPNN
## 2322	-18.50402374	0.667233806	1 2980	ThermoMPNN
## 2323	-13.29536724	0.234714442	0 2999	ThermoMPNN
## 2324	-11.62112398	-0.342799779	0 3580	ThermoMPNN
## 2325	-10.27467289	0.381256012	0 3581	ThermoMPNN
## 2326	-4.72669773	1.057955054	1 3582	ThermoMPNN
## 2327	-13.54102554	0.127019719	0 3589	ThermoMPNN

## 2328	-13.97968864	-0.540421933	0 3590	ThermoMPNN
## 2329	-14.08353100	0.256830928	0 3592	ThermoMPNN
## 2330	-11.48845596	-0.114557472	0 3583	ThermoMPNN
## 2331	-12.07261410	-0.067499338	0 3594	ThermoMPNN
## 2332	-8.47823763	-0.139063635	0 3595	ThermoMPNN
## 2333	-13.44969311	-0.029207743	0 3584	ThermoMPNN
## 2334	-12.43760567	-0.115554886	0 3593	ThermoMPNN
## 2335	-12.48370590	-0.360140409	0 3597	ThermoMPNN
## 2336	-11.36437073	-0.312343655	0 3599	ThermoMPNN
## 2337	-11.84329300	-0.236163907	0 3585	ThermoMPNN
## 2338	-12.64321690	0.196053023	0 3596	ThermoMPNN
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## 2340	-13.71621704	0.041859998	0 3601	ThermoMPNN
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## 2343	-13.33869305	-0.732454042	0 3604	ThermoMPNN
## 2344	-15.52120819	-0.484206043	0 3605	ThermoMPNN
## 2345	-18.54212914	-0.716277014	0 3606	ThermoMPNN
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## 2348	-9.79385586	0.596595371	1 3609	ThermoMPNN
## 2349	-10.86957245	0.421866771	0 3610	ThermoMPNN
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## 2351	-12.48058929	-0.214528460	0 3612	ThermoMPNN
## 2352	-18.25937920	-0.190910590	0 3613	ThermoMPNN
## 2353	-17.36299515	-0.305359517	0 3614	ThermoMPNN
## 2354	-14.54447250	-0.211734884	0 3615	ThermoMPNN
## 2355	-12.08109379	-0.614567523	0 3616	ThermoMPNN
## 2356	-18.34041252	-0.209608260	0 3618	ThermoMPNN
## 2357	-16.81215782	-0.310614470	0 3619	ThermoMPNN
## 2358	-7.99047937	0.797622678	1 3620	ThermoMPNN
## 2359	-13.15700760	0.873870819	1 3621	ThermoMPNN
## 2360	-12.41970882	-0.049604141	0 3623	ThermoMPNN
## 2361	-13.47637806	0.218882914	0 3624	ThermoMPNN
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## 2364	-9.63525553	0.238595144	0 3627	ThermoMPNN
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## 2367	-11.07718220	0.037071368	0 3630	ThermoMPNN
## 2368	-14.99263725	-0.489911607	0 3631	ThermoMPNN
## 2369	-13.62114925	0.347195317	0 3632	ThermoMPNN
## 2370	-14.98685703	-0.023193312	0 3634	ThermoMPNN
## 2371	-12.62735329	0.248954609	0 3635	ThermoMPNN
## 2372	-11.65318775	0.542801021	0 3636	ThermoMPNN
## 2373	-16.62861443	0.130771048	0 3638	ThermoMPNN
## 2374	-15.73357410	0.174992700	0 3639	ThermoMPNN
## 2375	-12.67615280	0.175816764	0 3659	ThermoMPNN
## 2376	-12.25289898	-0.413470818	0 3658	ThermoMPNN
## 2377	-9.00522728	0.112739087	0 3649	ThermoMPNN
## 2378	-8.48018064	0.049817391	0 3657	ThermoMPNN
## 2379	-10.81936035	-0.414202884	0 3647	ThermoMPNN
## 2380	-5.86793737	0.790768752	1 3640	ThermoMPNN
## 2381	-7.56519179	0.303651455	0 3655	ThermoMPNN

## 2382	-8.98102360	0.782298068	1 3651	ThermoMPNN
## 2383	-8.01954470	1.460760180	1 3656	ThermoMPNN
## 2384	-7.52637138	0.164638185	0 3648	ThermoMPNN
## 2385	-11.18040941	0.041592723	0 3652	ThermoMPNN
## 2386	-8.92810602	-0.647301580	0 3650	ThermoMPNN
## 2387	-8.66263647	1.982054703	1 3642	ThermoMPNN
## 2388	-9.94622822	0.554767135	0 3646	ThermoMPNN
## 2389	-12.23731747	-0.219295280	0 3644	ThermoMPNN
## 2390	-10.49935818	-0.039030124	0 3641	ThermoMPNN
## 2391	-6.50925722	3.188888420	1 3653	ThermoMPNN
## 2392	-8.26410074	0.277990387	0 3654	ThermoMPNN
## 2393	-6.94484711	0.923104853	1 3643	ThermoMPNN
## 2394	-14.23039227	-0.348431551	0 3679	ThermoMPNN
## 2395	-10.68446331	-0.147904234	0 3677	ThermoMPNN
## 2396	-14.72476883	-0.283713393	0 3678	ThermoMPNN
## 2397	-13.65805035	0.338528529	0 3660	ThermoMPNN
## 2398	-13.57716331	1.062443350	1 3661	ThermoMPNN
## 2399	-10.73846340	-0.131994390	0 3664	ThermoMPNN
## 2400	-14.97595596	-0.133824854	0 3671	ThermoMPNN
## 2401	-15.32314510	0.639617871	1 3662	ThermoMPNN
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## 2403	-12.45784855	-0.620496757	0 3674	ThermoMPNN
## 2404	-11.46463547	-0.118340194	0 3673	ThermoMPNN
## 2405	-8.49722919	0.542319488	0 3670	ThermoMPNN
## 2406	-13.06353931	-0.095830607	0 3675	ThermoMPNN
## 2407	-12.47075214	-0.204421817	0 3663	ThermoMPNN
## 2408	-13.00078430	-0.990289333	0 3666	ThermoMPNN
## 2409	-13.87660027	-0.102658813	0 3668	ThermoMPNN
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## 2411	-15.51833725	0.132653117	0 3665	ThermoMPNN
## 2412	-19.02190132	-0.444621702	0 3682	ThermoMPNN
## 2413	-16.09330006	0.087845269	0 3680	ThermoMPNN
## 2414	-15.61967945	-0.465946608	0 3695	ThermoMPNN
## 2415	-11.34324417	-0.168655841	0 3697	ThermoMPNN
## 2416	-15.94129429	-0.150173797	0 3696	ThermoMPNN
## 2417	-16.25416012	-0.286954703	0 3694	ThermoMPNN
## 2418	-17.87979584	-0.702043061	0 3688	ThermoMPNN
## 2419	-16.03599815	-0.225846410	0 3698	ThermoMPNN
## 2420	-11.79084129	0.235594145	0 3687	ThermoMPNN
## 2421	-15.00949211	-0.002275630	0 3681	ThermoMPNN
## 2422	-15.40205956	0.540655332	0 3693	ThermoMPNN
## 2423	-18.06464539	-0.067541366	0 3683	ThermoMPNN
## 2424	-17.97610321	-0.252684685	0 3685	ThermoMPNN
## 2425	-15.54319096	0.409410695	0 3699	ThermoMPNN
## 2426	-10.52059746	0.301676119	0 3690	ThermoMPNN
## 2427	-18.66141853	0.620745805	1 3691	ThermoMPNN
## 2428	-13.81974888	1.361584219	1 3692	ThermoMPNN
## 2429	-8.38935404	2.164313770	1 3708	ThermoMPNN
## 2430	-10.80950546	-0.121237328	0 3709	ThermoMPNN
## 2431	-15.84789410	-0.111380699	0 3712	ThermoMPNN
## 2432	-8.05399704	-0.312928103	0 3713	ThermoMPNN
## 2433	-11.04881229	-0.143834205	0 3711	ThermoMPNN
## 2434	-12.76134892	-0.174782164	0 3717	ThermoMPNN
## 2435	-11.51170502	0.158507493	0 3718	ThermoMPNN

## 2436	-11.06400642	0.347334436	0 3710	ThermoMPNN
## 2437	-14.41978874	-0.220109149	0 3704	ThermoMPNN
## 2438	-11.97030201	0.532675426	0 3705	ThermoMPNN
## 2439	-9.78531113	-0.135980325	0 3706	ThermoMPNN
## 2440	-11.99029293	-0.192202875	0 3707	ThermoMPNN
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## 2442	-9.93772287	0.165596852	0 3716	ThermoMPNN
## 2443	-12.06204290	0.109721929	0 3700	ThermoMPNN
## 2444	-10.48320713	-0.244619127	0 3701	ThermoMPNN
## 2445	-12.77278824	-0.778563943	0 3719	ThermoMPNN
## 2446	-12.74347954	0.005996459	0 3703	ThermoMPNN
## 2447	-15.50754185	1.549682760	1 3702	ThermoMPNN
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## 2449	-4.00697320	0.179898791	0 3723	ThermoMPNN
## 2450	-11.49740944	0.739150049	1 3726	ThermoMPNN
## 2451	-16.99995728	0.235253462	0 3732	ThermoMPNN
## 2452	-9.05048580	0.293854290	0 3731	ThermoMPNN
## 2453	-14.22549095	-0.384797748	0 3721	ThermoMPNN
## 2454	-8.89292345	0.764912789	1 3720	ThermoMPNN
## 2455	-9.36061792	0.237703904	0 3725	ThermoMPNN
## 2456	-11.34453945	-0.110154802	0 3736	ThermoMPNN
## 2457	-9.25365105	1.534271763	1 3733	ThermoMPNN
## 2458	-11.38743439	0.061679798	0 3734	ThermoMPNN
## 2459	-10.91430721	2.437481805	1 3735	ThermoMPNN
## 2460	-15.52078114	0.024393212	0 3724	ThermoMPNN
## 2461	-9.12805290	0.346667783	0 3728	ThermoMPNN
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## 2463	-13.26892262	0.473662492	0 3729	ThermoMPNN
## 2464	-11.58998871	0.012882331	0 3737	ThermoMPNN
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## 2467	-12.10478840	-0.660662904	0 3743	ThermoMPNN
## 2468	-12.79564362	-0.298756855	0 3741	ThermoMPNN
## 2469	-14.39648705	0.264692925	0 3752	ThermoMPNN
## 2470	-14.16002197	-0.315312896	0 3751	ThermoMPNN
## 2471	-15.96362114	-0.266402528	0 3759	ThermoMPNN
## 2472	-14.92297115	-0.454660236	0 3748	ThermoMPNN
## 2473	-10.06029530	0.405078192	0 3745	ThermoMPNN
## 2474	-15.71693344	-0.234667644	0 3753	ThermoMPNN
## 2475	-8.24578695	0.806502425	1 3755	ThermoMPNN
## 2476	-10.16612091	0.393835662	0 3756	ThermoMPNN
## 2477	-15.27398510	-0.616149286	0 3750	ThermoMPNN
## 2478	-16.21636925	1.083687430	1 3749	ThermoMPNN
## 2479	-15.20910931	-0.103776129	0 3754	ThermoMPNN
## 2480	-10.88013115	0.574546417	1 3757	ThermoMPNN
## 2481	-17.58879299	0.025029021	0 3758	ThermoMPNN
## 2482	-14.56599503	-0.277368159	0 3747	ThermoMPNN
## 2483	-16.37202339	-0.442282793	0 3746	ThermoMPNN
## 2484	-18.30372963	-0.300277001	0 3778	ThermoMPNN
## 2485	-14.64001865	-0.211103357	0 3775	ThermoMPNN
## 2486	-8.46111021	0.540027904	0 3777	ThermoMPNN
## 2487	-16.34269180	-0.359890889	0 3774	ThermoMPNN
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## 2492	-8.72832022	-0.173205298	0 3770	ThermoMPNN
## 2493	-13.47206821	-0.285523721	0 3760	ThermoMPNN
## 2494	-17.37092228	-0.259229613	0 3772	ThermoMPNN
## 2495	-11.67080040	-0.061659065	0 3764	ThermoMPNN
## 2496	-15.91745567	0.021612900	0 3768	ThermoMPNN
## 2497	-11.75185890	0.539598465	0 3776	ThermoMPNN
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## 2502	-13.40061264	0.728020499	1 3784	ThermoMPNN
## 2503	-6.65181665	0.923927658	1 3794	ThermoMPNN
## 2504	-10.11770058	1.537173437	1 3795	ThermoMPNN
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## 2511	-9.65987988	1.597572535	1 3791	ThermoMPNN
## 2512	-11.74071808	0.396282985	0 3781	ThermoMPNN
## 2513	-13.08723907	0.250908413	0 3798	ThermoMPNN
## 2514	-12.74273300	1.633578362	1 3799	ThermoMPNN
## 2515	-11.07380428	0.352376038	0 3789	ThermoMPNN
## 2516	-8.50116501	0.288889973	0 3793	ThermoMPNN
## 2517	-16.16928616	0.220505800	0 3792	ThermoMPNN
## 2518	-11.03581524	1.500505840	1 3780	ThermoMPNN
## 2519	-11.30245380	0.980575711	1 3806	ThermoMPNN
## 2520	-13.41267586	0.182774416	0 3807	ThermoMPNN
## 2521	-16.18458271	-0.217549723	0 3804	ThermoMPNN
## 2522	-11.79134274	-0.173999118	0 3801	ThermoMPNN
## 2523	-15.00213623	0.116061446	0 3802	ThermoMPNN
## 2524	-13.67467270	-0.451416078	0 3803	ThermoMPNN
## 2525	-12.40858727	-0.391636690	0 3805	ThermoMPNN
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## 2527	-14.46704845	-0.274836767	0 3817	ThermoMPNN
## 2528	-12.85197411	0.030119002	0 3818	ThermoMPNN
## 2529	-11.84757347	0.791762131	1 3815	ThermoMPNN
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## 2532	-12.95206547	0.014073590	0 3809	ThermoMPNN
## 2533	-14.86871853	-0.354707597	0 3819	ThermoMPNN
## 2534	-11.57178288	0.086414185	0 3811	ThermoMPNN
## 2535	-15.53521862	-0.832513068	0 3812	ThermoMPNN
## 2536	-11.00115833	-0.200478424	0 3813	ThermoMPNN
## 2537	-12.69855347	-0.105819880	0 3810	ThermoMPNN
## 2538	-14.18189182	0.102595842	0 3837	ThermoMPNN
## 2539	-12.40845909	0.166807576	0 3831	ThermoMPNN
## 2540	-10.68427086	-0.350262697	0 3833	ThermoMPNN
## 2541	-11.51909790	0.123966440	0 3835	ThermoMPNN
## 2542	-13.39922943	1.185823608	1 3836	ThermoMPNN
## 2543	-16.31959724	0.309408115	0 3832	ThermoMPNN

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## 2545	-13.46013622	-0.472482163	0 3839	ThermoMPNN
## 2546	-15.25714149	0.259912897	0 3823	ThermoMPNN
## 2547	-14.15403366	0.471494674	0 3820	ThermoMPNN
## 2548	-13.97729301	0.068275783	0 3827	ThermoMPNN
## 2549	-9.31706553	0.368289865	0 3828	ThermoMPNN
## 2550	-12.82228127	0.655160607	1 3829	ThermoMPNN
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## 2552	-15.41079578	-0.162868799	0 3824	ThermoMPNN
## 2553	-10.80337906	0.219833908	0 3821	ThermoMPNN
## 2554	-16.00818596	0.185981082	0 3822	ThermoMPNN
## 2555	-13.29478149	0.065503313	0 3825	ThermoMPNN
## 2556	-10.59244804	2.589555783	1 3826	ThermoMPNN
## 2557	-10.35736599	-0.196649860	0 3857	ThermoMPNN
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## 2561	-8.77478113	0.288420551	0 3840	ThermoMPNN
## 2562	-13.70807667	0.255925647	0 3858	ThermoMPNN
## 2563	-10.10395813	0.934226112	1 3851	ThermoMPNN
## 2564	-13.43219509	1.161359951	1 3850	ThermoMPNN
## 2565	-9.56826344	0.008935364	0 3854	ThermoMPNN
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## 2568	-13.51170082	0.466056437	0 3849	ThermoMPNN
## 2569	-14.38188267	0.413709471	0 3847	ThermoMPNN
## 2570	-11.41367264	0.528222437	0 3853	ThermoMPNN
## 2571	-12.05495872	0.955997907	1 3846	ThermoMPNN
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## 2578	-14.14826031	-0.539779149	0 3868	ThermoMPNN
## 2579	-15.49739056	0.889678770	1 3869	ThermoMPNN
## 2580	-16.06559181	1.745474248	1 3864	ThermoMPNN
## 2581	-13.43966179	0.021705594	0 3877	ThermoMPNN
## 2582	-15.37681255	0.038869818	0 3874	ThermoMPNN
## 2583	-10.72567215	0.513046492	0 3865	ThermoMPNN
## 2584	-12.88629436	1.024169648	1 3875	ThermoMPNN
## 2585	-8.98699894	1.043515604	1 3863	ThermoMPNN
## 2586	-17.67400703	-0.522437012	0 3878	ThermoMPNN
## 2587	-13.73521461	-0.138713165	0 3879	ThermoMPNN
## 2588	-15.31074314	1.535052856	1 3867	ThermoMPNN
## 2589	-14.96277008	0.505379290	0 3861	ThermoMPNN
## 2590	-15.64443836	0.365054553	0 3872	ThermoMPNN
## 2591	-12.55385742	0.005408942	0 3866	ThermoMPNN
## 2592	-12.36818180	1.833301464	1 3860	ThermoMPNN
## 2593	-9.39866276	1.102170622	1 3897	ThermoMPNN
## 2594	-12.93387470	0.156746867	0 3891	ThermoMPNN
## 2595	-15.12599583	2.050912621	1 3888	ThermoMPNN
## 2596	-14.99811535	-0.475038509	0 3892	ThermoMPNN
## 2597	-12.09163551	-0.246289886	0 3895	ThermoMPNN

## 2598	-14.22332478	0.307199567	0 3893	ThermoMPNN
## 2599	-14.02622738	0.100005101	0 3894	ThermoMPNN
## 2600	-9.23012342	0.897703319	1 3887	ThermoMPNN
## 2601	-12.26345253	-0.206316315	0 3896	ThermoMPNN
## 2602	-11.30324631	0.812836628	1 3886	ThermoMPNN
## 2603	-13.25441608	-0.029637682	0 3880	ThermoMPNN
## 2604	-14.90181389	0.024176639	0 3882	ThermoMPNN
## 2605	-8.36985681	0.468643286	0 3889	ThermoMPNN
## 2606	-10.84440374	-0.116322595	0 3890	ThermoMPNN
## 2607	-14.12903118	-0.096344616	0 3898	ThermoMPNN
## 2608	-15.77258911	-0.437416833	0 3883	ThermoMPNN
## 2609	-15.04224644	-0.019950181	0 3885	ThermoMPNN
## 2610	-8.09436960	0.053036777	0 3899	ThermoMPNN
## 2611	-14.87066479	0.198617830	0 3912	ThermoMPNN
## 2612	-13.88342762	-0.057870693	0 3909	ThermoMPNN
## 2613	-9.97202854	-0.461720873	0 3911	ThermoMPNN
## 2614	-13.32195644	1.096567894	1 3907	ThermoMPNN
## 2615	-13.19370193	0.880338687	1 3919	ThermoMPNN
## 2616	-13.27710133	2.055554321	1 3914	ThermoMPNN
## 2617	-12.11136265	0.927727642	1 3915	ThermoMPNN
## 2618	-9.45851574	1.183046425	1 3913	ThermoMPNN
## 2619	-10.99026337	0.133867287	0 3905	ThermoMPNN
## 2620	-16.44326134	0.595785260	1 3918	ThermoMPNN
## 2621	-15.43925800	0.022977846	0 3904	ThermoMPNN
## 2622	-12.43118935	-0.116114965	0 3916	ThermoMPNN
## 2623	-13.39442978	0.248815717	0 3910	ThermoMPNN
## 2624	-10.79178104	0.535539030	0 3906	ThermoMPNN
## 2625	-14.33894958	1.768653041	1 3901	ThermoMPNN
## 2626	-11.49420719	0.862509889	1 3900	ThermoMPNN
## 2627	-11.27180405	0.127288389	0 3917	ThermoMPNN
## 2628	-9.26655102	1.495965748	1 3929	ThermoMPNN
## 2629	-16.41436272	0.255163882	0 3931	ThermoMPNN
## 2630	-16.28208733	0.362384011	0 3925	ThermoMPNN
## 2631	-6.73885069	1.287656969	1 3927	ThermoMPNN
## 2632	-17.27767525	-0.125861497	0 3923	ThermoMPNN
## 2633	-18.15223656	-0.554559674	0 3922	ThermoMPNN
## 2634	-17.95981407	-0.454970239	0 3926	ThermoMPNN
## 2635	-16.63457298	0.150040156	0 3933	ThermoMPNN
## 2636	-11.14858246	0.341603429	0 3936	ThermoMPNN
## 2637	-17.32379456	-0.155770031	0 3939	ThermoMPNN
## 2638	-15.45580235	-0.045567615	0 3932	ThermoMPNN
## 2639	-13.04758263	2.170968606	1 3920	ThermoMPNN
## 2640	-15.24068222	1.074499737	1 3935	ThermoMPNN
## 2641	-17.94457741	-0.111954426	0 3938	ThermoMPNN
## 2642	-16.09011765	-0.102328306	0 3934	ThermoMPNN
## 2643	-8.30026655	2.470780566	1 3937	ThermoMPNN
## 2644	-11.86310081	0.676953084	1 3946	ThermoMPNN
## 2645	-12.42355995	2.413499860	1 3953	ThermoMPNN
## 2646	-13.11565704	1.507732703	1 3954	ThermoMPNN
## 2647	-10.40271778	-0.103153809	0 3945	ThermoMPNN
## 2648	-16.14452953	0.508260327	0 3944	ThermoMPNN
## 2649	-15.43191891	0.536392329	0 3949	ThermoMPNN
## 2650	-13.05596905	2.679371399	1 3948	ThermoMPNN
## 2651	-11.43153477	0.518176167	0 3955	ThermoMPNN

##	2652	-8.05676146	2.104850520	1	3943	ThermoMPNN
##	2653	-17.06792412	0.796939489	1	3958	ThermoMPNN
##	2654	-14.01195793	1.519588404	1	3956	ThermoMPNN
##	2655	-15.24717083	1.668007383	1	3950	ThermoMPNN
##	2656	-16.27165184	0.210414662	0	3952	ThermoMPNN
##	2657	-14.07636395	0.668136799	1	3957	ThermoMPNN
##	2658	-16.29389458	0.822080911	1	3947	ThermoMPNN
##	2659	-12.40037575	1.059773828	1	3940	ThermoMPNN
##	2660	-9.49680119	0.780540403	1	3951	ThermoMPNN
##	2661	-14.03861370	0.114555529	0	3941	ThermoMPNN
##	2662	-9.51949368	-0.122195114	0	3960	ThermoMPNN
##	2663	-11.36610165	0.083088195	0	3961	ThermoMPNN
##	2664	-15.51228313	-0.075356645	0	3963	ThermoMPNN
##	2665	-13.83108597	-0.033281292	0	3965	ThermoMPNN
##	2666	-16.54135647	-0.261768032	0	3966	ThermoMPNN
##	2667	-6.82646103	-0.128647343	0	3967	ThermoMPNN
##	2668	-16.56419544	-0.152217978	0	3968	ThermoMPNN
##	2669	-9.16742086	-0.090920048	0	3969	ThermoMPNN
##	2670	-9.36942120	-0.479106022	0	3970	ThermoMPNN
##	2671	-14.08706665	-0.143571458	0	3971	ThermoMPNN
##	2672	-13.85159760	-0.268337092	0	3972	ThermoMPNN
##	2673	-16.35837440	0.031615151	0	3973	ThermoMPNN
##	2674	-15.67565823	-0.124100422	0	3974	ThermoMPNN
##	2675	-12.68109951	0.265659772	0	3975	ThermoMPNN
##	2676	-10.85930920	-0.356606406	0	3976	ThermoMPNN
##	2677	-17.76320724	-0.295142642	0	3978	ThermoMPNN
##	2678	-15.32604237	-0.651058132	0	3979	ThermoMPNN
##	2679	-7.78802338	-0.181991076	0	3980	ThermoMPNN
##	2680	-9.44112720	1.192037223	1	3981	ThermoMPNN
##	2681	-13.07654057	0.311015267	0	3983	ThermoMPNN
##	2682	-10.48217764	-0.000307989	0	3984	ThermoMPNN
##	2683	-12.13280716	0.230045984	0	3985	ThermoMPNN
##	2684	-13.09812717	-0.140207564	0	3986	ThermoMPNN
##	2685	-8.46345415	0.381082072	0	3987	ThermoMPNN
##	2686	-14.52812443	-0.503206574	0	3988	ThermoMPNN
##	2687	-8.49242630	0.612735007	1	3989	ThermoMPNN
##	2688	-9.26506004	0.110165756	0	3990	ThermoMPNN
##	2689	-13.13141232	-0.131570151	0	3991	ThermoMPNN
##	2690	-14.30021858	0.215710953	0	3992	ThermoMPNN
##	2691	-11.99698753	-0.309632929	0	3993	ThermoMPNN
##	2692	-12.53403378	0.381828223	0	3994	ThermoMPNN
##	2693	-9.83682652	0.246229325	0	3995	ThermoMPNN
##	2694	-9.31564283	0.401739122	0	3996	ThermoMPNN
##	2695	-14.69721355	0.190890317	0	3998	ThermoMPNN
##	2696	-11.25704708	-0.203753193	0	3999	ThermoMPNN
##	2697	-10.48318138	0.079328826	0	4016	ThermoMPNN
##	2698	-17.47735558	0.154140919	0	4013	ThermoMPNN
##	2699	-18.02808418	-0.707386828	0	4019	ThermoMPNN
##	2700	-16.55608368	-0.533453640	0	4014	ThermoMPNN
##	2701	-15.93755989	-0.014756301	0	4009	ThermoMPNN
##	2702	-18.09796600	-0.113184668	0	4006	ThermoMPNN
##		Dataset	ddG_pred	position	wildtype	mutation
##	1	AF-P35557-F1-model_v2	0.401084542	13	E	F
##	2	AF-P35557-F1-model_v2	0.225024819	13	E	K

## 3	AF-P35557-F1-model_v2	0.546358109	13	E	N
## 4	AF-P35557-F1-model_v2	0.416388035	13	E	D
## 5	AF-P35557-F1-model_v2	0.214462280	13	E	R
## 6	AF-P35557-F1-model_v2	0.765403152	13	E	G
## 7	AF-P35557-F1-model_v2	0.161455870	13	E	L
## 8	AF-P35557-F1-model_v2	0.065832138	13	E	C
## 9	AF-P35557-F1-model_v2	0.136145949	13	E	M
## 10	AF-P35557-F1-model_v2	0.261531651	13	E	I
## 11	AF-P35557-F1-model_v2	0.377307951	13	E	S
## 12	AF-P35557-F1-model_v2	0.138719738	13	E	Q
## 13	AF-P35557-F1-model_v2	0.424748421	13	E	H
## 14	AF-P35557-F1-model_v2	0.311345041	13	E	Y
## 15	AF-P35557-F1-model_v2	0.473424792	13	E	T
## 16	AF-P35557-F1-model_v2	1.984701157	13	E	P
## 17	AF-P35557-F1-model_v2	0.058123589	13	E	A
## 18	AF-P35557-F1-model_v2	0.214265585	13	E	W
## 19	AF-P35557-F1-model_v2	0.388426304	13	E	V
## 20	AF-P35557-F1-model_v2	0.408344030	14	K	A
## 21	AF-P35557-F1-model_v2	0.821419418	14	K	W
## 22	AF-P35557-F1-model_v2	0.922816932	14	K	Y
## 23	AF-P35557-F1-model_v2	0.887028754	14	K	V
## 24	AF-P35557-F1-model_v2	0.293606758	14	K	Q
## 25	AF-P35557-F1-model_v2	0.654321015	14	K	C
## 26	AF-P35557-F1-model_v2	0.834105194	14	K	S
## 27	AF-P35557-F1-model_v2	0.988797903	14	K	T
## 28	AF-P35557-F1-model_v2	0.381281495	14	K	M
## 29	AF-P35557-F1-model_v2	0.876404345	14	K	E
## 30	AF-P35557-F1-model_v2	1.350611210	14	K	G
## 31	AF-P35557-F1-model_v2	1.477392316	14	K	D
## 32	AF-P35557-F1-model_v2	0.655767858	14	K	I
## 33	AF-P35557-F1-model_v2	2.814215422	14	K	P
## 34	AF-P35557-F1-model_v2	0.939313531	14	K	F
## 35	AF-P35557-F1-model_v2	-0.042739868	14	K	R
## 36	AF-P35557-F1-model_v2	0.443498969	14	K	L
## 37	AF-P35557-F1-model_v2	0.807597458	14	K	H
## 38	AF-P35557-F1-model_v2	1.236492395	15	V	A
## 39	AF-P35557-F1-model_v2	2.550171852	15	V	D
## 40	AF-P35557-F1-model_v2	2.166349649	15	V	E
## 41	AF-P35557-F1-model_v2	1.233297586	15	V	F
## 42	AF-P35557-F1-model_v2	2.412172079	15	V	G
## 43	AF-P35557-F1-model_v2	2.180015087	15	V	H
## 44	AF-P35557-F1-model_v2	0.116993904	15	V	I
## 45	AF-P35557-F1-model_v2	2.112286568	15	V	K
## 46	AF-P35557-F1-model_v2	0.850274920	15	V	L
## 47	AF-P35557-F1-model_v2	1.010402441	15	V	M
## 48	AF-P35557-F1-model_v2	2.499843121	15	V	N
## 49	AF-P35557-F1-model_v2	2.399929285	15	V	P
## 50	AF-P35557-F1-model_v2	2.001850367	15	V	Q
## 51	AF-P35557-F1-model_v2	2.094366074	15	V	R
## 52	AF-P35557-F1-model_v2	1.873124719	15	V	S
## 53	AF-P35557-F1-model_v2	1.313356876	15	V	T
## 54	AF-P35557-F1-model_v2	1.391653538	15	V	W
## 55	AF-P35557-F1-model_v2	1.513029218	15	V	Y
## 56	AF-P35557-F1-model_v2	2.289705753	16	E	P

## 57	AF-P35557-F1-model_v2	0.335174799	16	E	Q
## 58	AF-P35557-F1-model_v2	0.700693190	16	E	H
## 59	AF-P35557-F1-model_v2	1.018950939	16	E	G
## 60	AF-P35557-F1-model_v2	0.715376854	16	E	Y
## 61	AF-P35557-F1-model_v2	0.320702076	16	E	L
## 62	AF-P35557-F1-model_v2	0.557568371	16	E	N
## 63	AF-P35557-F1-model_v2	0.649387658	16	E	I
## 64	AF-P35557-F1-model_v2	0.694905400	16	E	K
## 65	AF-P35557-F1-model_v2	0.786321998	16	E	F
## 66	AF-P35557-F1-model_v2	0.681144893	16	E	S
## 67	AF-P35557-F1-model_v2	0.735962987	16	E	R
## 68	AF-P35557-F1-model_v2	0.885162175	16	E	T
## 69	AF-P35557-F1-model_v2	0.693163812	16	E	W
## 70	AF-P35557-F1-model_v2	0.293701053	16	E	D
## 71	AF-P35557-F1-model_v2	0.389874458	16	E	A
## 72	AF-P35557-F1-model_v2	0.828931332	16	E	V
## 73	AF-P35557-F1-model_v2	0.301916242	16	E	C
## 74	AF-P35557-F1-model_v2	0.266444266	17	Q	E
## 75	AF-P35557-F1-model_v2	0.083052278	17	Q	C
## 76	AF-P35557-F1-model_v2	0.636664212	17	Q	D
## 77	AF-P35557-F1-model_v2	0.235466003	17	Q	V
## 78	AF-P35557-F1-model_v2	0.254697919	17	Q	Y
## 79	AF-P35557-F1-model_v2	0.457935989	17	Q	N
## 80	AF-P35557-F1-model_v2	0.674811125	17	Q	G
## 81	AF-P35557-F1-model_v2	0.257111430	17	Q	H
## 82	AF-P35557-F1-model_v2	0.213445723	17	Q	W
## 83	AF-P35557-F1-model_v2	0.232976198	17	Q	T
## 84	AF-P35557-F1-model_v2	0.062736154	17	Q	M
## 85	AF-P35557-F1-model_v2	2.052599669	17	Q	P
## 86	AF-P35557-F1-model_v2	-0.077521682	17	Q	R
## 87	AF-P35557-F1-model_v2	0.313177049	17	Q	F
## 88	AF-P35557-F1-model_v2	0.094243348	17	Q	A
## 89	AF-P35557-F1-model_v2	0.119701147	17	Q	L
## 90	AF-P35557-F1-model_v2	0.266263187	17	Q	S
## 91	AF-P35557-F1-model_v2	-0.024821639	17	Q	K
## 92	AF-P35557-F1-model_v2	0.116979659	17	Q	I
## 93	AF-P35557-F1-model_v2	1.735247493	18	I	T
## 94	AF-P35557-F1-model_v2	2.178588390	18	I	S
## 95	AF-P35557-F1-model_v2	1.079369187	18	I	C
## 96	AF-P35557-F1-model_v2	0.602847576	18	I	V
## 97	AF-P35557-F1-model_v2	2.420751810	18	I	N
## 98	AF-P35557-F1-model_v2	1.724256277	18	I	A
## 99	AF-P35557-F1-model_v2	1.204289198	18	I	W
## 100	AF-P35557-F1-model_v2	2.062634945	18	I	R
## 101	AF-P35557-F1-model_v2	2.321234941	18	I	E
## 102	AF-P35557-F1-model_v2	0.358057022	18	I	L
## 103	AF-P35557-F1-model_v2	2.141548872	18	I	Q
## 104	AF-P35557-F1-model_v2	2.633857965	18	I	D
## 105	AF-P35557-F1-model_v2	1.941179633	18	I	H
## 106	AF-P35557-F1-model_v2	0.857313395	18	I	F
## 107	AF-P35557-F1-model_v2	2.066252470	18	I	K
## 108	AF-P35557-F1-model_v2	0.853831291	18	I	M
## 109	AF-P35557-F1-model_v2	1.103653312	18	I	Y
## 110	AF-P35557-F1-model_v2	2.435302496	18	I	G

## 111	AF-P35557-F1-model_v2	1.130939007	19	L	F
## 112	AF-P35557-F1-model_v2	2.010791779	19	L	T
## 113	AF-P35557-F1-model_v2	1.866848230	19	L	W
## 114	AF-P35557-F1-model_v2	1.120133162	19	L	I
## 115	AF-P35557-F1-model_v2	2.416750431	19	L	G
## 116	AF-P35557-F1-model_v2	2.480503798	19	L	E
## 117	AF-P35557-F1-model_v2	2.427868843	19	L	H
## 118	AF-P35557-F1-model_v2	2.333991766	19	L	S
## 119	AF-P35557-F1-model_v2	2.355313778	19	L	K
## 120	AF-P35557-F1-model_v2	2.480403423	19	L	D
## 121	AF-P35557-F1-model_v2	2.359813690	19	L	N
## 122	AF-P35557-F1-model_v2	1.264382958	19	L	C
## 123	AF-P35557-F1-model_v2	2.409818411	19	L	R
## 124	AF-P35557-F1-model_v2	2.205513477	19	L	A
## 125	AF-P35557-F1-model_v2	1.537369370	19	L	V
## 126	AF-P35557-F1-model_v2	2.408489704	19	L	Q
## 127	AF-P35557-F1-model_v2	0.986274004	19	L	M
## 128	AF-P35557-F1-model_v2	1.845116019	19	L	Y
## 129	AF-P35557-F1-model_v2	2.622858286	19	L	P
## 130	AF-P35557-F1-model_v2	0.297477007	20	A	L
## 131	AF-P35557-F1-model_v2	0.146397948	20	A	K
## 132	AF-P35557-F1-model_v2	0.638611615	20	A	E
## 133	AF-P35557-F1-model_v2	1.756692529	20	A	P
## 134	AF-P35557-F1-model_v2	0.426682830	20	A	I
## 135	AF-P35557-F1-model_v2	0.632131577	20	A	G
## 136	AF-P35557-F1-model_v2	0.817372918	20	A	D
## 137	AF-P35557-F1-model_v2	0.274414539	20	A	C
## 138	AF-P35557-F1-model_v2	0.230094373	20	A	M
## 139	AF-P35557-F1-model_v2	0.512947559	20	A	H
## 140	AF-P35557-F1-model_v2	0.123735905	20	A	R
## 141	AF-P35557-F1-model_v2	0.576496720	20	A	V
## 142	AF-P35557-F1-model_v2	0.307200909	20	A	Q
## 143	AF-P35557-F1-model_v2	0.519383848	20	A	Y
## 144	AF-P35557-F1-model_v2	0.486687839	20	A	W
## 145	AF-P35557-F1-model_v2	0.570069551	20	A	N
## 146	AF-P35557-F1-model_v2	0.291418850	20	A	S
## 147	AF-P35557-F1-model_v2	0.580121934	20	A	T
## 148	AF-P35557-F1-model_v2	0.755446911	21	E	D
## 149	AF-P35557-F1-model_v2	0.200050831	21	E	A
## 150	AF-P35557-F1-model_v2	0.522859335	21	E	Y
## 151	AF-P35557-F1-model_v2	0.593325853	21	E	W
## 152	AF-P35557-F1-model_v2	0.233494282	21	E	L
## 153	AF-P35557-F1-model_v2	0.502589762	21	E	H
## 154	AF-P35557-F1-model_v2	0.070152879	21	E	C
## 155	AF-P35557-F1-model_v2	0.476698160	21	E	G
## 156	AF-P35557-F1-model_v2	0.471187890	21	E	F
## 157	AF-P35557-F1-model_v2	0.211026192	21	E	M
## 158	AF-P35557-F1-model_v2	0.407128930	21	E	K
## 159	AF-P35557-F1-model_v2	0.737715125	21	E	T
## 160	AF-P35557-F1-model_v2	0.481558502	21	E	R
## 161	AF-P35557-F1-model_v2	0.681404829	21	E	N
## 162	AF-P35557-F1-model_v2	0.600391090	21	E	V
## 163	AF-P35557-F1-model_v2	0.612642288	21	E	S
## 164	AF-P35557-F1-model_v2	0.111876369	21	E	Q

## 165	AF-P35557-F1-model_v2	0.509227931	21	E	I
## 166	AF-P35557-F1-model_v2	0.646959424	22	F	W
## 167	AF-P35557-F1-model_v2	1.090139031	22	F	L
## 168	AF-P35557-F1-model_v2	1.505443573	22	F	V
## 169	AF-P35557-F1-model_v2	1.549566031	22	F	H
## 170	AF-P35557-F1-model_v2	2.263097763	22	F	G
## 171	AF-P35557-F1-model_v2	1.299319029	22	F	M
## 172	AF-P35557-F1-model_v2	2.213724613	22	F	K
## 173	AF-P35557-F1-model_v2	2.087394953	22	F	N
## 174	AF-P35557-F1-model_v2	2.466569185	22	F	D
## 175	AF-P35557-F1-model_v2	2.146404743	22	F	S
## 176	AF-P35557-F1-model_v2	2.082844734	22	F	T
## 177	AF-P35557-F1-model_v2	1.983405709	22	F	A
## 178	AF-P35557-F1-model_v2	1.032587051	22	F	C
## 179	AF-P35557-F1-model_v2	2.168318033	22	F	R
## 180	AF-P35557-F1-model_v2	2.177827358	22	F	Q
## 181	AF-P35557-F1-model_v2	2.001586199	22	F	P
## 182	AF-P35557-F1-model_v2	0.087900519	23	Q	F
## 183	AF-P35557-F1-model_v2	0.144861758	23	Q	E
## 184	AF-P35557-F1-model_v2	0.050522804	23	Q	L
## 185	AF-P35557-F1-model_v2	0.870624721	23	Q	G
## 186	AF-P35557-F1-model_v2	-0.061107397	23	Q	I
## 187	AF-P35557-F1-model_v2	0.222354949	23	Q	K
## 188	AF-P35557-F1-model_v2	0.106270075	23	Q	Y
## 189	AF-P35557-F1-model_v2	-0.035772085	23	Q	C
## 190	AF-P35557-F1-model_v2	0.073507071	23	Q	M
## 191	AF-P35557-F1-model_v2	0.068666577	23	Q	W
## 192	AF-P35557-F1-model_v2	0.254574418	23	Q	A
## 193	AF-P35557-F1-model_v2	0.192263782	23	Q	R
## 194	AF-P35557-F1-model_v2	0.285312533	23	Q	S
## 195	AF-P35557-F1-model_v2	0.130911291	23	Q	T
## 196	AF-P35557-F1-model_v2	2.059420824	23	Q	P
## 197	AF-P35557-F1-model_v2	-0.063946724	23	Q	V
## 198	AF-P35557-F1-model_v2	2.140776157	24	L	N
## 199	AF-P35557-F1-model_v2	2.262980938	24	L	P
## 200	AF-P35557-F1-model_v2	2.391168118	24	L	D
## 201	AF-P35557-F1-model_v2	2.325634003	24	L	G
## 202	AF-P35557-F1-model_v2	0.348806620	24	L	F
## 203	AF-P35557-F1-model_v2	0.624438405	24	L	M
## 204	AF-P35557-F1-model_v2	1.976422071	24	L	Q
## 205	AF-P35557-F1-model_v2	2.198906183	24	L	E
## 206	AF-P35557-F1-model_v2	0.608359575	24	L	I
## 207	AF-P35557-F1-model_v2	2.074937344	24	L	R
## 208	AF-P35557-F1-model_v2	1.976207256	24	L	S
## 209	AF-P35557-F1-model_v2	1.600071430	24	L	T
## 210	AF-P35557-F1-model_v2	0.953323007	24	L	C
## 211	AF-P35557-F1-model_v2	0.539083362	24	L	W
## 212	AF-P35557-F1-model_v2	0.548050404	24	L	Y
## 213	AF-P35557-F1-model_v2	1.702470064	24	L	H
## 214	AF-P35557-F1-model_v2	0.924204826	24	L	V
## 215	AF-P35557-F1-model_v2	2.097358465	24	L	K
## 216	AF-P35557-F1-model_v2	1.912995577	24	L	A
## 217	AF-P35557-F1-model_v2	-0.017682791	25	Q	A
## 218	AF-P35557-F1-model_v2	-0.055883706	25	Q	C

## 219	AF-P35557-F1-model_v2	0.379321218	25	Q	D
## 220	AF-P35557-F1-model_v2	0.416331857	25	Q	F
## 221	AF-P35557-F1-model_v2	0.268162489	25	Q	M
## 222	AF-P35557-F1-model_v2	0.037226856	25	Q	N
## 223	AF-P35557-F1-model_v2	0.305420518	25	Q	E
## 224	AF-P35557-F1-model_v2	0.039949656	25	Q	R
## 225	AF-P35557-F1-model_v2	-0.524951816	25	Q	S
## 226	AF-P35557-F1-model_v2	-0.611065388	25	Q	T
## 227	AF-P35557-F1-model_v2	0.354084700	25	Q	P
## 228	AF-P35557-F1-model_v2	-0.097423911	25	Q	K
## 229	AF-P35557-F1-model_v2	0.247401774	25	Q	L
## 230	AF-P35557-F1-model_v2	0.194341481	25	Q	G
## 231	AF-P35557-F1-model_v2	0.554500580	25	Q	Y
## 232	AF-P35557-F1-model_v2	0.391975284	25	Q	V
## 233	AF-P35557-F1-model_v2	0.745646954	25	Q	W
## 234	AF-P35557-F1-model_v2	0.301514983	25	Q	I
## 235	AF-P35557-F1-model_v2	1.177285910	26	E	K
## 236	AF-P35557-F1-model_v2	-0.059555113	26	E	F
## 237	AF-P35557-F1-model_v2	0.715228558	26	E	S
## 238	AF-P35557-F1-model_v2	-0.350925148	26	E	L
## 239	AF-P35557-F1-model_v2	1.013279080	26	E	N
## 240	AF-P35557-F1-model_v2	1.185695529	26	E	R
## 241	AF-P35557-F1-model_v2	-0.469644248	26	E	I
## 242	AF-P35557-F1-model_v2	0.105104685	26	E	Y
## 243	AF-P35557-F1-model_v2	0.010404229	26	E	C
## 244	AF-P35557-F1-model_v2	-0.048634589	26	E	V
## 245	AF-P35557-F1-model_v2	0.477507383	26	E	T
## 246	AF-P35557-F1-model_v2	-0.082430065	26	E	W
## 247	AF-P35557-F1-model_v2	0.680427313	26	E	A
## 248	AF-P35557-F1-model_v2	0.680290937	26	E	P
## 249	AF-P35557-F1-model_v2	-0.015520215	26	E	M
## 250	AF-P35557-F1-model_v2	1.250994444	26	E	G
## 251	AF-P35557-F1-model_v2	0.665323615	26	E	Q
## 252	AF-P35557-F1-model_v2	0.709397435	26	E	H
## 253	AF-P35557-F1-model_v2	0.193845034	27	E	Q
## 254	AF-P35557-F1-model_v2	0.594603717	27	E	P
## 255	AF-P35557-F1-model_v2	0.224905610	27	E	V
## 256	AF-P35557-F1-model_v2	0.012475729	27	E	A
## 257	AF-P35557-F1-model_v2	0.227852225	27	E	N
## 258	AF-P35557-F1-model_v2	0.335216641	27	E	K
## 259	AF-P35557-F1-model_v2	0.248775959	27	E	I
## 260	AF-P35557-F1-model_v2	0.083365202	27	E	S
## 261	AF-P35557-F1-model_v2	0.256337583	27	E	W
## 262	AF-P35557-F1-model_v2	0.344520330	27	E	M
## 263	AF-P35557-F1-model_v2	0.343959570	27	E	T
## 264	AF-P35557-F1-model_v2	0.237216234	27	E	H
## 265	AF-P35557-F1-model_v2	0.463580608	27	E	G
## 266	AF-P35557-F1-model_v2	0.064970851	27	E	C
## 267	AF-P35557-F1-model_v2	0.252487063	27	E	L
## 268	AF-P35557-F1-model_v2	0.442584097	27	E	F
## 269	AF-P35557-F1-model_v2	-0.022824228	27	E	D
## 270	AF-P35557-F1-model_v2	0.355832696	27	E	R
## 271	AF-P35557-F1-model_v2	0.346181035	27	E	Y
## 272	AF-P35557-F1-model_v2	1.021554470	28	D	S

## 273	AF-P35557-F1-model_v2	-0.291897893	28	D	Q
## 274	AF-P35557-F1-model_v2	0.774205863	28	D	C
## 275	AF-P35557-F1-model_v2	1.666117549	28	D	R
## 276	AF-P35557-F1-model_v2	0.918771386	28	D	L
## 277	AF-P35557-F1-model_v2	1.325111628	28	D	V
## 278	AF-P35557-F1-model_v2	1.013128519	28	D	T
## 279	AF-P35557-F1-model_v2	-0.019294739	28	D	E
## 280	AF-P35557-F1-model_v2	1.484248281	28	D	K
## 281	AF-P35557-F1-model_v2	1.219069004	28	D	I
## 282	AF-P35557-F1-model_v2	0.784618318	28	D	A
## 283	AF-P35557-F1-model_v2	3.658584118	28	D	P
## 284	AF-P35557-F1-model_v2	0.349391580	28	D	M
## 285	AF-P35557-F1-model_v2	1.373221517	28	D	F
## 286	AF-P35557-F1-model_v2	1.066863060	28	D	W
## 287	AF-P35557-F1-model_v2	1.588892460	28	D	G
## 288	AF-P35557-F1-model_v2	2.552035332	29	L	R
## 289	AF-P35557-F1-model_v2	2.342990875	29	L	Q
## 290	AF-P35557-F1-model_v2	1.609672666	29	L	C
## 291	AF-P35557-F1-model_v2	3.197623491	29	L	P
## 292	AF-P35557-F1-model_v2	2.670382261	29	L	A
## 293	AF-P35557-F1-model_v2	3.317108154	29	L	G
## 294	AF-P35557-F1-model_v2	2.867728710	29	L	S
## 295	AF-P35557-F1-model_v2	2.936220646	29	L	N
## 296	AF-P35557-F1-model_v2	2.569620848	29	L	Y
## 297	AF-P35557-F1-model_v2	2.591943026	29	L	E
## 298	AF-P35557-F1-model_v2	2.646166563	29	L	T
## 299	AF-P35557-F1-model_v2	3.145664454	29	L	D
## 300	AF-P35557-F1-model_v2	2.213052034	29	L	F
## 301	AF-P35557-F1-model_v2	2.369171143	29	L	K
## 302	AF-P35557-F1-model_v2	2.336014748	29	L	W
## 303	AF-P35557-F1-model_v2	2.831451416	29	L	H
## 304	AF-P35557-F1-model_v2	1.635987878	29	L	V
## 305	AF-P35557-F1-model_v2	1.204322696	29	L	I
## 306	AF-P35557-F1-model_v2	0.246526778	30	K	Y
## 307	AF-P35557-F1-model_v2	0.307071030	30	K	W
## 308	AF-P35557-F1-model_v2	0.490924776	30	K	T
## 309	AF-P35557-F1-model_v2	0.458781540	30	K	A
## 310	AF-P35557-F1-model_v2	-0.041247725	30	K	V
## 311	AF-P35557-F1-model_v2	0.824747801	30	K	S
## 312	AF-P35557-F1-model_v2	1.317310333	30	K	D
## 313	AF-P35557-F1-model_v2	0.877688885	30	K	N
## 314	AF-P35557-F1-model_v2	0.272078693	30	K	F
## 315	AF-P35557-F1-model_v2	0.014521003	30	K	C
## 316	AF-P35557-F1-model_v2	2.438329220	30	K	P
## 317	AF-P35557-F1-model_v2	-0.196056247	30	K	I
## 318	AF-P35557-F1-model_v2	0.472579718	30	K	E
## 319	AF-P35557-F1-model_v2	-0.007719874	30	K	R
## 320	AF-P35557-F1-model_v2	0.151946545	30	K	Q
## 321	AF-P35557-F1-model_v2	-0.200822592	30	K	L
## 322	AF-P35557-F1-model_v2	1.262455225	30	K	G
## 323	AF-P35557-F1-model_v2	0.438260019	30	K	H
## 324	AF-P35557-F1-model_v2	0.158828318	31	K	S
## 325	AF-P35557-F1-model_v2	-0.043053985	31	K	R
## 326	AF-P35557-F1-model_v2	-0.085741997	31	K	T

## 327	AF-P35557-F1-model_v2	0.869030058	31	K	G
## 328	AF-P35557-F1-model_v2	0.077348471	31	K	A
## 329	AF-P35557-F1-model_v2	-0.163535893	31	K	C
## 330	AF-P35557-F1-model_v2	-0.518220782	31	K	V
## 331	AF-P35557-F1-model_v2	0.378420115	31	K	D
## 332	AF-P35557-F1-model_v2	0.123417377	31	K	H
## 333	AF-P35557-F1-model_v2	-0.570302129	31	K	I
## 334	AF-P35557-F1-model_v2	-0.002072811	31	K	Y
## 335	AF-P35557-F1-model_v2	-0.006359160	31	K	Q
## 336	AF-P35557-F1-model_v2	0.001015842	31	K	E
## 337	AF-P35557-F1-model_v2	0.036499381	31	K	F
## 338	AF-P35557-F1-model_v2	0.064657688	31	K	W
## 339	AF-P35557-F1-model_v2	-0.195842743	31	K	L
## 340	AF-P35557-F1-model_v2	-0.082374811	31	K	M
## 341	AF-P35557-F1-model_v2	1.771588206	31	K	P
## 342	AF-P35557-F1-model_v2	1.539611578	32	V	A
## 343	AF-P35557-F1-model_v2	0.973201990	32	V	C
## 344	AF-P35557-F1-model_v2	2.487505913	32	V	E
## 345	AF-P35557-F1-model_v2	1.198766947	32	V	F
## 346	AF-P35557-F1-model_v2	2.418459892	32	V	G
## 347	AF-P35557-F1-model_v2	2.279570103	32	V	H
## 348	AF-P35557-F1-model_v2	-0.579578876	32	V	I
## 349	AF-P35557-F1-model_v2	2.307081223	32	V	K
## 350	AF-P35557-F1-model_v2	0.128942847	32	V	L
## 351	AF-P35557-F1-model_v2	0.858237386	32	V	M
## 352	AF-P35557-F1-model_v2	2.402079344	32	V	N
## 353	AF-P35557-F1-model_v2	2.357842445	32	V	P
## 354	AF-P35557-F1-model_v2	2.357720852	32	V	Q
## 355	AF-P35557-F1-model_v2	2.351717949	32	V	R
## 356	AF-P35557-F1-model_v2	2.374258995	32	V	S
## 357	AF-P35557-F1-model_v2	1.895197630	32	V	T
## 358	AF-P35557-F1-model_v2	1.549646378	32	V	W
## 359	AF-P35557-F1-model_v2	1.586642385	32	V	Y
## 360	AF-P35557-F1-model_v2	2.469602346	33	M	P
## 361	AF-P35557-F1-model_v2	2.525411844	33	M	N
## 362	AF-P35557-F1-model_v2	2.004933596	33	M	E
## 363	AF-P35557-F1-model_v2	1.954691291	33	M	H
## 364	AF-P35557-F1-model_v2	0.494891524	33	M	L
## 365	AF-P35557-F1-model_v2	0.745731831	33	M	C
## 366	AF-P35557-F1-model_v2	2.616981506	33	M	G
## 367	AF-P35557-F1-model_v2	1.449241400	33	M	Q
## 368	AF-P35557-F1-model_v2	1.131104708	33	M	Y
## 369	AF-P35557-F1-model_v2	1.792450547	33	M	S
## 370	AF-P35557-F1-model_v2	0.603544950	33	M	V
## 371	AF-P35557-F1-model_v2	0.809076071	33	M	W
## 372	AF-P35557-F1-model_v2	1.311644912	33	M	A
## 373	AF-P35557-F1-model_v2	1.714427948	33	M	T
## 374	AF-P35557-F1-model_v2	2.011664867	33	M	R
## 375	AF-P35557-F1-model_v2	2.694184303	33	M	D
## 376	AF-P35557-F1-model_v2	1.135710835	34	R	G
## 377	AF-P35557-F1-model_v2	1.126533985	35	R	C
## 378	AF-P35557-F1-model_v2	1.079010963	35	R	A
## 379	AF-P35557-F1-model_v2	1.387633443	35	R	S
## 380	AF-P35557-F1-model_v2	1.470207572	35	R	T

## 381	AF-P35557-F1-model_v2	3.078538179	35	R	P
## 382	AF-P35557-F1-model_v2	1.262750506	35	R	Q
## 383	AF-P35557-F1-model_v2	1.980226159	35	R	G
## 384	AF-P35557-F1-model_v2	1.368423939	35	R	H
## 385	AF-P35557-F1-model_v2	1.946638107	35	R	E
## 386	AF-P35557-F1-model_v2	1.225403309	35	R	F
## 387	AF-P35557-F1-model_v2	0.510729313	35	R	L
## 388	AF-P35557-F1-model_v2	0.680699348	35	R	M
## 389	AF-P35557-F1-model_v2	1.584830046	35	R	N
## 390	AF-P35557-F1-model_v2	0.877001762	35	R	I
## 391	AF-P35557-F1-model_v2	0.552883983	35	R	K
## 392	AF-P35557-F1-model_v2	1.185600162	35	R	V
## 393	AF-P35557-F1-model_v2	1.216902018	35	R	Y
## 394	AF-P35557-F1-model_v2	1.586629868	36	M	Y
## 395	AF-P35557-F1-model_v2	2.889548540	36	M	D
## 396	AF-P35557-F1-model_v2	1.021314859	36	M	V
## 397	AF-P35557-F1-model_v2	1.651950121	36	M	W
## 398	AF-P35557-F1-model_v2	2.547530174	36	M	E
## 399	AF-P35557-F1-model_v2	0.408769965	36	M	F
## 400	AF-P35557-F1-model_v2	1.955738187	36	M	A
## 401	AF-P35557-F1-model_v2	1.256992221	36	M	C
## 402	AF-P35557-F1-model_v2	2.559205770	36	M	S
## 403	AF-P35557-F1-model_v2	2.150624752	36	M	T
## 404	AF-P35557-F1-model_v2	0.336265206	36	M	I
## 405	AF-P35557-F1-model_v2	2.659512043	36	M	R
## 406	AF-P35557-F1-model_v2	2.344505548	36	M	Q
## 407	AF-P35557-F1-model_v2	2.542940140	36	M	H
## 408	AF-P35557-F1-model_v2	-0.254611015	36	M	L
## 409	AF-P35557-F1-model_v2	2.580178976	36	M	G
## 410	AF-P35557-F1-model_v2	2.642683268	36	M	N
## 411	AF-P35557-F1-model_v2	2.676171064	36	M	P
## 412	AF-P35557-F1-model_v2	0.587417841	37	Q	C
## 413	AF-P35557-F1-model_v2	1.710417747	37	Q	G
## 414	AF-P35557-F1-model_v2	2.390974998	37	Q	D
## 415	AF-P35557-F1-model_v2	1.453230143	37	Q	E
## 416	AF-P35557-F1-model_v2	0.916326284	37	Q	A
## 417	AF-P35557-F1-model_v2	1.037544489	37	Q	S
## 418	AF-P35557-F1-model_v2	0.759381652	37	Q	T
## 419	AF-P35557-F1-model_v2	1.208426476	37	Q	F
## 420	AF-P35557-F1-model_v2	1.251215577	37	Q	W
## 421	AF-P35557-F1-model_v2	1.420369744	37	Q	Y
## 422	AF-P35557-F1-model_v2	1.056736231	37	Q	H
## 423	AF-P35557-F1-model_v2	0.376253128	37	Q	V
## 424	AF-P35557-F1-model_v2	3.181883097	37	Q	P
## 425	AF-P35557-F1-model_v2	-0.147565365	37	Q	R
## 426	AF-P35557-F1-model_v2	0.435868144	37	Q	L
## 427	AF-P35557-F1-model_v2	0.033305407	37	Q	M
## 428	AF-P35557-F1-model_v2	0.115014791	37	Q	I
## 429	AF-P35557-F1-model_v2	-0.094351888	37	Q	K
## 430	AF-P35557-F1-model_v2	1.452927589	37	Q	N
## 431	AF-P35557-F1-model_v2	-0.098879457	38	K	V
## 432	AF-P35557-F1-model_v2	-0.251233816	38	K	W
## 433	AF-P35557-F1-model_v2	-0.076218545	38	K	F
## 434	AF-P35557-F1-model_v2	0.175748885	38	K	T

## 435	AF-P35557-F1-model_v2	0.051115334	38	K	H
## 436	AF-P35557-F1-model_v2	-0.480735302	38	K	E
## 437	AF-P35557-F1-model_v2	0.456974089	38	K	G
## 438	AF-P35557-F1-model_v2	0.095020652	38	K	D
## 439	AF-P35557-F1-model_v2	-0.225897431	38	K	M
## 440	AF-P35557-F1-model_v2	0.249456793	38	K	N
## 441	AF-P35557-F1-model_v2	-0.279089928	38	K	Y
## 442	AF-P35557-F1-model_v2	-0.339241385	38	K	C
## 443	AF-P35557-F1-model_v2	-0.277726769	38	K	I
## 444	AF-P35557-F1-model_v2	-0.289162993	38	K	L
## 445	AF-P35557-F1-model_v2	0.144099832	38	K	S
## 446	AF-P35557-F1-model_v2	1.657212615	38	K	P
## 447	AF-P35557-F1-model_v2	-0.035888314	38	K	R
## 448	AF-P35557-F1-model_v2	-0.299543202	38	K	A
## 449	AF-P35557-F1-model_v2	-0.141945541	38	K	Q
## 450	AF-P35557-F1-model_v2	1.982585430	39	E	K
## 451	AF-P35557-F1-model_v2	1.309388876	39	E	H
## 452	AF-P35557-F1-model_v2	1.486657500	39	E	G
## 453	AF-P35557-F1-model_v2	1.793800473	39	E	F
## 454	AF-P35557-F1-model_v2	0.844648719	39	E	M
## 455	AF-P35557-F1-model_v2	1.338529229	39	E	I
## 456	AF-P35557-F1-model_v2	1.449570417	39	E	N
## 457	AF-P35557-F1-model_v2	1.209913611	39	E	L
## 458	AF-P35557-F1-model_v2	1.806362271	39	E	P
## 459	AF-P35557-F1-model_v2	0.724257588	39	E	A
## 460	AF-P35557-F1-model_v2	0.711250901	39	E	D
## 461	AF-P35557-F1-model_v2	1.930627108	39	E	R
## 462	AF-P35557-F1-model_v2	0.965592563	39	E	C
## 463	AF-P35557-F1-model_v2	1.213168859	39	E	S
## 464	AF-P35557-F1-model_v2	1.557785153	39	E	Y
## 465	AF-P35557-F1-model_v2	1.604562521	39	E	W
## 466	AF-P35557-F1-model_v2	1.395784497	39	E	T
## 467	AF-P35557-F1-model_v2	1.184093952	39	E	V
## 468	AF-P35557-F1-model_v2	2.776477337	40	M	D
## 469	AF-P35557-F1-model_v2	1.595570087	40	M	C
## 470	AF-P35557-F1-model_v2	2.589301586	40	M	E
## 471	AF-P35557-F1-model_v2	2.412845612	40	M	G
## 472	AF-P35557-F1-model_v2	2.393474579	40	M	T
## 473	AF-P35557-F1-model_v2	1.088820815	40	M	F
## 474	AF-P35557-F1-model_v2	1.980200768	40	M	A
## 475	AF-P35557-F1-model_v2	2.211146355	40	M	R
## 476	AF-P35557-F1-model_v2	2.536496162	40	M	S
## 477	AF-P35557-F1-model_v2	1.592467666	40	M	V
## 478	AF-P35557-F1-model_v2	1.753771782	40	M	W
## 479	AF-P35557-F1-model_v2	1.973800659	40	M	Q
## 480	AF-P35557-F1-model_v2	1.657582760	40	M	Y
## 481	AF-P35557-F1-model_v2	2.269824982	40	M	H
## 482	AF-P35557-F1-model_v2	0.002189875	40	M	L
## 483	AF-P35557-F1-model_v2	2.903407097	40	M	P
## 484	AF-P35557-F1-model_v2	0.816702187	41	D	V
## 485	AF-P35557-F1-model_v2	0.867738187	41	D	S
## 486	AF-P35557-F1-model_v2	2.706364155	41	D	P
## 487	AF-P35557-F1-model_v2	0.710319042	41	D	M
## 488	AF-P35557-F1-model_v2	0.689294636	41	D	Q

## 489	AF-P35557-F1-model_v2	0.971251428	41	D	W
## 490	AF-P35557-F1-model_v2	0.991312981	41	D	Y
## 491	AF-P35557-F1-model_v2	1.027106285	41	D	K
## 492	AF-P35557-F1-model_v2	0.585522532	41	D	L
## 493	AF-P35557-F1-model_v2	1.039833307	41	D	R
## 494	AF-P35557-F1-model_v2	0.570125341	41	D	N
## 495	AF-P35557-F1-model_v2	0.352841020	41	D	C
## 496	AF-P35557-F1-model_v2	0.781296313	41	D	I
## 497	AF-P35557-F1-model_v2	0.797146618	41	D	A
## 498	AF-P35557-F1-model_v2	1.257380724	41	D	G
## 499	AF-P35557-F1-model_v2	0.895515978	41	D	F
## 500	AF-P35557-F1-model_v2	0.980638146	41	D	T
## 501	AF-P35557-F1-model_v2	0.196418524	41	D	E
## 502	AF-P35557-F1-model_v2	1.921617508	42	R	A
## 503	AF-P35557-F1-model_v2	3.334216118	42	R	P
## 504	AF-P35557-F1-model_v2	1.047063351	42	R	L
## 505	AF-P35557-F1-model_v2	1.327076435	42	R	M
## 506	AF-P35557-F1-model_v2	1.985548258	42	R	N
## 507	AF-P35557-F1-model_v2	2.804914951	42	R	E
## 508	AF-P35557-F1-model_v2	2.185867071	42	R	S
## 509	AF-P35557-F1-model_v2	1.851589441	42	R	C
## 510	AF-P35557-F1-model_v2	2.981140137	42	R	D
## 511	AF-P35557-F1-model_v2	1.789966822	42	R	I
## 512	AF-P35557-F1-model_v2	0.823473811	42	R	K
## 513	AF-P35557-F1-model_v2	1.714880824	42	R	F
## 514	AF-P35557-F1-model_v2	2.830444336	42	R	G
## 515	AF-P35557-F1-model_v2	2.176103830	42	R	T
## 516	AF-P35557-F1-model_v2	2.253983259	42	R	V
## 517	AF-P35557-F1-model_v2	1.953090549	42	R	H
## 518	AF-P35557-F1-model_v2	1.838835001	42	R	Y
## 519	AF-P35557-F1-model_v2	1.894725800	42	R	W
## 520	AF-P35557-F1-model_v2	2.656029940	43	G	K
## 521	AF-P35557-F1-model_v2	2.241213322	43	G	I
## 522	AF-P35557-F1-model_v2	2.346606493	43	G	H
## 523	AF-P35557-F1-model_v2	1.838602066	43	G	F
## 524	AF-P35557-F1-model_v2	1.830262423	43	G	A
## 525	AF-P35557-F1-model_v2	2.110049963	43	G	M
## 526	AF-P35557-F1-model_v2	1.886938930	43	G	Y
## 527	AF-P35557-F1-model_v2	1.866672039	43	G	W
## 528	AF-P35557-F1-model_v2	2.110820293	43	G	V
## 529	AF-P35557-F1-model_v2	2.743248940	43	G	E
## 530	AF-P35557-F1-model_v2	2.250041485	43	G	L
## 531	AF-P35557-F1-model_v2	2.342091322	43	G	T
## 532	AF-P35557-F1-model_v2	2.228075743	43	G	S
## 533	AF-P35557-F1-model_v2	2.315603495	43	G	P
## 534	AF-P35557-F1-model_v2	2.421245813	43	G	R
## 535	AF-P35557-F1-model_v2	2.547307730	43	G	N
## 536	AF-P35557-F1-model_v2	2.547740936	43	G	Q
## 537	AF-P35557-F1-model_v2	2.284654856	44	L	S
## 538	AF-P35557-F1-model_v2	2.018720865	44	L	T
## 539	AF-P35557-F1-model_v2	2.215463638	44	L	A
## 540	AF-P35557-F1-model_v2	1.679427147	44	L	R
## 541	AF-P35557-F1-model_v2	2.839480877	44	L	D
## 542	AF-P35557-F1-model_v2	1.944958448	44	L	W

## 543	AF-P35557-F1-model_v2	1.539120317	44	L	C
## 544	AF-P35557-F1-model_v2	1.365830541	44	L	I
## 545	AF-P35557-F1-model_v2	1.613002181	44	L	V
## 546	AF-P35557-F1-model_v2	2.039069653	44	L	Q
## 547	AF-P35557-F1-model_v2	2.495849133	44	L	H
## 548	AF-P35557-F1-model_v2	2.429498911	44	L	G
## 549	AF-P35557-F1-model_v2	2.552757978	44	L	E
## 550	AF-P35557-F1-model_v2	2.941862822	44	L	P
## 551	AF-P35557-F1-model_v2	1.805024385	44	L	K
## 552	AF-P35557-F1-model_v2	2.243003368	44	L	Y
## 553	AF-P35557-F1-model_v2	2.506522894	44	L	N
## 554	AF-P35557-F1-model_v2	2.407765388	45	R	E
## 555	AF-P35557-F1-model_v2	1.335527897	45	R	A
## 556	AF-P35557-F1-model_v2	1.320690989	45	R	C
## 557	AF-P35557-F1-model_v2	2.139012098	45	R	D
## 558	AF-P35557-F1-model_v2	1.619385958	45	R	T
## 559	AF-P35557-F1-model_v2	3.298631191	45	R	P
## 560	AF-P35557-F1-model_v2	1.568572164	45	R	Q
## 561	AF-P35557-F1-model_v2	1.195362687	45	R	S
## 562	AF-P35557-F1-model_v2	1.177428603	45	R	H
## 563	AF-P35557-F1-model_v2	1.823161364	45	R	V
## 564	AF-P35557-F1-model_v2	1.591540813	45	R	F
## 565	AF-P35557-F1-model_v2	2.028695822	45	R	G
## 566	AF-P35557-F1-model_v2	1.442261457	45	R	M
## 567	AF-P35557-F1-model_v2	0.924379468	45	R	N
## 568	AF-P35557-F1-model_v2	1.655661345	45	R	I
## 569	AF-P35557-F1-model_v2	0.656381726	45	R	K
## 570	AF-P35557-F1-model_v2	2.027391195	45	R	W
## 571	AF-P35557-F1-model_v2	1.669560313	45	R	Y
## 572	AF-P35557-F1-model_v2	1.394487858	45	R	L
## 573	AF-P35557-F1-model_v2	0.427357078	46	L	H
## 574	AF-P35557-F1-model_v2	0.771521866	46	L	G
## 575	AF-P35557-F1-model_v2	0.314194202	46	L	Y
## 576	AF-P35557-F1-model_v2	0.511046529	46	L	W
## 577	AF-P35557-F1-model_v2	-0.301562309	46	L	K
## 578	AF-P35557-F1-model_v2	-0.129899383	46	L	I
## 579	AF-P35557-F1-model_v2	1.166370749	46	L	D
## 580	AF-P35557-F1-model_v2	0.816042542	46	L	E
## 581	AF-P35557-F1-model_v2	0.287519813	46	L	F
## 582	AF-P35557-F1-model_v2	0.090984404	46	L	V
## 583	AF-P35557-F1-model_v2	0.328891754	46	L	T
## 584	AF-P35557-F1-model_v2	0.398671389	46	L	Q
## 585	AF-P35557-F1-model_v2	1.008870840	46	L	P
## 586	AF-P35557-F1-model_v2	-0.543570280	46	L	R
## 587	AF-P35557-F1-model_v2	0.148711205	46	L	M
## 588	AF-P35557-F1-model_v2	0.112681627	46	L	A
## 589	AF-P35557-F1-model_v2	0.273424685	46	L	S
## 590	AF-P35557-F1-model_v2	0.639604270	46	L	N
## 591	AF-P35557-F1-model_v2	0.121720731	46	L	C
## 592	AF-P35557-F1-model_v2	0.284454644	47	E	N
## 593	AF-P35557-F1-model_v2	0.135757148	47	E	S
## 594	AF-P35557-F1-model_v2	0.050718009	47	E	D
## 595	AF-P35557-F1-model_v2	0.383083999	47	E	L
## 596	AF-P35557-F1-model_v2	0.537723064	47	E	P

## 597	AF-P35557-F1-model_v2	0.340634346	47	E	G
## 598	AF-P35557-F1-model_v2	0.325578213	47	E	H
## 599	AF-P35557-F1-model_v2	0.461711109	47	E	I
## 600	AF-P35557-F1-model_v2	0.460702240	47	E	R
## 601	AF-P35557-F1-model_v2	0.389265418	47	E	T
## 602	AF-P35557-F1-model_v2	0.480393648	47	E	V
## 603	AF-P35557-F1-model_v2	0.048358440	47	E	A
## 604	AF-P35557-F1-model_v2	1.134902716	48	T	A
## 605	AF-P35557-F1-model_v2	0.760723591	48	T	C
## 606	AF-P35557-F1-model_v2	1.283488154	48	T	D
## 607	AF-P35557-F1-model_v2	1.236604929	48	T	E
## 608	AF-P35557-F1-model_v2	0.864580870	48	T	F
## 609	AF-P35557-F1-model_v2	1.349433780	48	T	G
## 610	AF-P35557-F1-model_v2	1.045843601	48	T	H
## 611	AF-P35557-F1-model_v2	1.131645203	48	T	I
## 612	AF-P35557-F1-model_v2	1.300185204	48	T	K
## 613	AF-P35557-F1-model_v2	0.926521480	48	T	L
## 614	AF-P35557-F1-model_v2	1.095262527	48	T	M
## 615	AF-P35557-F1-model_v2	0.940657735	48	T	N
## 616	AF-P35557-F1-model_v2	1.624210477	48	T	P
## 617	AF-P35557-F1-model_v2	1.213955641	48	T	Q
## 618	AF-P35557-F1-model_v2	1.303741455	48	T	R
## 619	AF-P35557-F1-model_v2	0.635293245	48	T	S
## 620	AF-P35557-F1-model_v2	1.024542809	48	T	V
## 621	AF-P35557-F1-model_v2	0.773483217	48	T	W
## 622	AF-P35557-F1-model_v2	1.383963585	49	H	D
## 623	AF-P35557-F1-model_v2	-0.154302478	49	H	A
## 624	AF-P35557-F1-model_v2	1.604409695	49	H	E
## 625	AF-P35557-F1-model_v2	0.058869362	49	H	C
## 626	AF-P35557-F1-model_v2	0.192498207	49	H	V
## 627	AF-P35557-F1-model_v2	0.419561267	49	H	R
## 628	AF-P35557-F1-model_v2	0.743867874	49	H	W
## 629	AF-P35557-F1-model_v2	0.616977155	49	H	F
## 630	AF-P35557-F1-model_v2	0.874649882	49	H	I
## 631	AF-P35557-F1-model_v2	0.324799001	49	H	T
## 632	AF-P35557-F1-model_v2	0.774842799	49	H	Q
## 633	AF-P35557-F1-model_v2	0.733269036	49	H	G
## 634	AF-P35557-F1-model_v2	0.384800136	49	H	Y
## 635	AF-P35557-F1-model_v2	0.855035245	49	H	M
## 636	AF-P35557-F1-model_v2	0.799466491	49	H	K
## 637	AF-P35557-F1-model_v2	0.120321631	49	H	S
## 638	AF-P35557-F1-model_v2	0.852162242	49	H	P
## 639	AF-P35557-F1-model_v2	1.157204151	49	H	L
## 640	AF-P35557-F1-model_v2	0.378933191	50	E	M
## 641	AF-P35557-F1-model_v2	0.283997655	50	E	K
## 642	AF-P35557-F1-model_v2	0.365950167	50	E	R
## 643	AF-P35557-F1-model_v2	0.277764201	50	E	H
## 644	AF-P35557-F1-model_v2	0.362392426	50	E	L
## 645	AF-P35557-F1-model_v2	0.468969584	50	E	W
## 646	AF-P35557-F1-model_v2	0.430996656	50	E	I
## 647	AF-P35557-F1-model_v2	0.295429051	50	E	S
## 648	AF-P35557-F1-model_v2	0.431620061	50	E	T
## 649	AF-P35557-F1-model_v2	0.523227155	50	E	V
## 650	AF-P35557-F1-model_v2	0.121476710	50	E	A

## 651	AF-P35557-F1-model_v2	0.327058613	50	E	G
## 652	AF-P35557-F1-model_v2	0.334107876	50	E	N
## 653	AF-P35557-F1-model_v2	0.364142776	50	E	P
## 654	AF-P35557-F1-model_v2	0.192803562	50	E	Q
## 655	AF-P35557-F1-model_v2	0.426690340	50	E	F
## 656	AF-P35557-F1-model_v2	0.314876854	50	E	Y
## 657	AF-P35557-F1-model_v2	0.125999510	50	E	C
## 658	AF-P35557-F1-model_v2	0.025795698	51	E	R
## 659	AF-P35557-F1-model_v2	-0.020766079	51	E	K
## 660	AF-P35557-F1-model_v2	-0.009593308	51	E	Y
## 661	AF-P35557-F1-model_v2	0.071730256	51	E	L
## 662	AF-P35557-F1-model_v2	-0.080826700	51	E	Q
## 663	AF-P35557-F1-model_v2	-0.047714829	51	E	T
## 664	AF-P35557-F1-model_v2	-0.020884991	51	E	W
## 665	AF-P35557-F1-model_v2	0.055130124	51	E	M
## 666	AF-P35557-F1-model_v2	0.139994144	51	E	I
## 667	AF-P35557-F1-model_v2	-0.051504433	51	E	S
## 668	AF-P35557-F1-model_v2	1.174108982	51	E	P
## 669	AF-P35557-F1-model_v2	-0.239255428	51	E	C
## 670	AF-P35557-F1-model_v2	-0.035001099	51	E	H
## 671	AF-P35557-F1-model_v2	0.135181308	51	E	G
## 672	AF-P35557-F1-model_v2	-0.004498065	51	E	A
## 673	AF-P35557-F1-model_v2	0.034878790	51	E	D
## 674	AF-P35557-F1-model_v2	-0.047397852	51	E	F
## 675	AF-P35557-F1-model_v2	0.187439561	51	E	V
## 676	AF-P35557-F1-model_v2	1.902369618	52	A	H
## 677	AF-P35557-F1-model_v2	1.240427494	52	A	M
## 678	AF-P35557-F1-model_v2	1.362004519	52	A	L
## 679	AF-P35557-F1-model_v2	1.196722984	52	A	T
## 680	AF-P35557-F1-model_v2	1.421018243	52	A	W
## 681	AF-P35557-F1-model_v2	0.814365864	52	A	V
## 682	AF-P35557-F1-model_v2	1.801166296	52	A	Q
## 683	AF-P35557-F1-model_v2	1.319203019	52	A	G
## 684	AF-P35557-F1-model_v2	1.890707374	52	A	N
## 685	AF-P35557-F1-model_v2	1.373773098	52	A	P
## 686	AF-P35557-F1-model_v2	1.792425871	52	A	K
## 687	AF-P35557-F1-model_v2	1.247608542	52	A	I
## 688	AF-P35557-F1-model_v2	0.821061015	52	A	S
## 689	AF-P35557-F1-model_v2	0.741214752	52	A	C
## 690	AF-P35557-F1-model_v2	1.798080683	52	A	E
## 691	AF-P35557-F1-model_v2	1.299040079	52	A	F
## 692	AF-P35557-F1-model_v2	1.526090384	52	A	Y
## 693	AF-P35557-F1-model_v2	1.771287322	52	A	R
## 694	AF-P35557-F1-model_v2	0.324313641	53	S	A
## 695	AF-P35557-F1-model_v2	0.661886454	53	S	C
## 696	AF-P35557-F1-model_v2	1.022203684	53	S	D
## 697	AF-P35557-F1-model_v2	1.560731053	53	S	E
## 698	AF-P35557-F1-model_v2	1.619366765	53	S	F
## 699	AF-P35557-F1-model_v2	1.007067442	53	S	G
## 700	AF-P35557-F1-model_v2	1.570265293	53	S	H
## 701	AF-P35557-F1-model_v2	1.534571767	53	S	I
## 702	AF-P35557-F1-model_v2	1.928376317	53	S	K
## 703	AF-P35557-F1-model_v2	1.657356977	53	S	L
## 704	AF-P35557-F1-model_v2	1.320881367	53	S	M

## 705	AF-P35557-F1-model_v2	0.835058808	53	S	P
## 706	AF-P35557-F1-model_v2	1.413162231	53	S	Q
## 707	AF-P35557-F1-model_v2	1.767445207	53	S	R
## 708	AF-P35557-F1-model_v2	0.076296210	53	S	T
## 709	AF-P35557-F1-model_v2	1.015574217	53	S	V
## 710	AF-P35557-F1-model_v2	1.536640286	53	S	W
## 711	AF-P35557-F1-model_v2	1.693630934	53	S	Y
## 712	AF-P35557-F1-model_v2	1.445818424	54	V	A
## 713	AF-P35557-F1-model_v2	0.919336796	54	V	C
## 714	AF-P35557-F1-model_v2	2.627593040	54	V	E
## 715	AF-P35557-F1-model_v2	1.999778867	54	V	G
## 716	AF-P35557-F1-model_v2	2.180863142	54	V	H
## 717	AF-P35557-F1-model_v2	2.200083971	54	V	K
## 718	AF-P35557-F1-model_v2	1.040586233	54	V	L
## 719	AF-P35557-F1-model_v2	1.560389996	54	V	M
## 720	AF-P35557-F1-model_v2	2.212973595	54	V	N
## 721	AF-P35557-F1-model_v2	2.350986004	54	V	P
## 722	AF-P35557-F1-model_v2	2.388062954	54	V	Q
## 723	AF-P35557-F1-model_v2	2.219040394	54	V	R
## 724	AF-P35557-F1-model_v2	1.902785063	54	V	S
## 725	AF-P35557-F1-model_v2	1.307751179	54	V	T
## 726	AF-P35557-F1-model_v2	1.819560766	54	V	W
## 727	AF-P35557-F1-model_v2	1.692290545	54	V	Y
## 728	AF-P35557-F1-model_v2	-0.049982429	55	K	R
## 729	AF-P35557-F1-model_v2	1.510077834	55	K	S
## 730	AF-P35557-F1-model_v2	0.948137522	55	K	Q
## 731	AF-P35557-F1-model_v2	1.581263185	55	K	G
## 732	AF-P35557-F1-model_v2	0.703835249	55	K	C
## 733	AF-P35557-F1-model_v2	2.313764095	55	K	E
## 734	AF-P35557-F1-model_v2	0.919130564	55	K	F
## 735	AF-P35557-F1-model_v2	1.276109695	55	K	A
## 736	AF-P35557-F1-model_v2	1.670080900	55	K	P
## 737	AF-P35557-F1-model_v2	1.029511333	55	K	H
## 738	AF-P35557-F1-model_v2	2.665464640	55	K	D
## 739	AF-P35557-F1-model_v2	2.135812998	55	K	T
## 740	AF-P35557-F1-model_v2	1.930599213	55	K	V
## 741	AF-P35557-F1-model_v2	0.826108217	55	K	W
## 742	AF-P35557-F1-model_v2	1.633846283	55	K	I
## 743	AF-P35557-F1-model_v2	0.795600653	55	K	L
## 744	AF-P35557-F1-model_v2	0.913584650	55	K	Y
## 745	AF-P35557-F1-model_v2	1.519819617	56	M	H
## 746	AF-P35557-F1-model_v2	1.070390224	56	M	I
## 747	AF-P35557-F1-model_v2	1.981848001	56	M	G
## 748	AF-P35557-F1-model_v2	1.426129341	56	M	W
## 749	AF-P35557-F1-model_v2	1.295434952	56	M	F
## 750	AF-P35557-F1-model_v2	1.817603350	56	M	N
## 751	AF-P35557-F1-model_v2	2.499943733	56	M	P
## 752	AF-P35557-F1-model_v2	0.268454313	56	M	L
## 753	AF-P35557-F1-model_v2	1.705875874	56	M	E
## 754	AF-P35557-F1-model_v2	1.176889777	56	M	A
## 755	AF-P35557-F1-model_v2	0.454043269	56	M	C
## 756	AF-P35557-F1-model_v2	1.625876784	56	M	Y
## 757	AF-P35557-F1-model_v2	2.249459505	56	M	D
## 758	AF-P35557-F1-model_v2	1.552571535	56	M	T

## 759	AF-P35557-F1-model_v2	1.001999259	56	M	V
## 760	AF-P35557-F1-model_v2	2.233350039	56	M	R
## 761	AF-P35557-F1-model_v2	1.559659719	56	M	S
## 762	AF-P35557-F1-model_v2	1.166519523	56	M	Q
## 763	AF-P35557-F1-model_v2	2.259023190	57	L	A
## 764	AF-P35557-F1-model_v2	1.408182859	57	L	C
## 765	AF-P35557-F1-model_v2	2.424851179	57	L	E
## 766	AF-P35557-F1-model_v2	2.857373238	57	L	P
## 767	AF-P35557-F1-model_v2	2.411629200	57	L	D
## 768	AF-P35557-F1-model_v2	2.249639511	57	L	K
## 769	AF-P35557-F1-model_v2	2.295614719	57	L	N
## 770	AF-P35557-F1-model_v2	2.399344921	57	L	Q
## 771	AF-P35557-F1-model_v2	2.052087784	57	L	R
## 772	AF-P35557-F1-model_v2	0.605632901	57	L	I
## 773	AF-P35557-F1-model_v2	2.408218622	57	L	S
## 774	AF-P35557-F1-model_v2	1.894785523	57	L	T
## 775	AF-P35557-F1-model_v2	1.354220152	57	L	V
## 776	AF-P35557-F1-model_v2	0.970088840	57	L	F
## 777	AF-P35557-F1-model_v2	2.796199799	57	L	G
## 778	AF-P35557-F1-model_v2	2.166564226	57	L	H
## 779	AF-P35557-F1-model_v2	1.238486052	57	L	Y
## 780	AF-P35557-F1-model_v2	1.436178207	57	L	W
## 781	AF-P35557-F1-model_v2	2.185723543	58	P	K
## 782	AF-P35557-F1-model_v2	1.545363188	58	P	M
## 783	AF-P35557-F1-model_v2	2.254134417	58	P	N
## 784	AF-P35557-F1-model_v2	2.358193874	58	P	Q
## 785	AF-P35557-F1-model_v2	1.258437276	58	P	L
## 786	AF-P35557-F1-model_v2	1.448933125	58	P	F
## 787	AF-P35557-F1-model_v2	2.123235464	58	P	G
## 788	AF-P35557-F1-model_v2	2.204233408	58	P	H
## 789	AF-P35557-F1-model_v2	2.342668533	58	P	R
## 790	AF-P35557-F1-model_v2	1.458824873	58	P	W
## 791	AF-P35557-F1-model_v2	2.073476791	58	P	S
## 792	AF-P35557-F1-model_v2	2.132639170	58	P	T
## 793	AF-P35557-F1-model_v2	1.328290462	58	P	I
## 794	AF-P35557-F1-model_v2	1.329919934	58	P	V
## 795	AF-P35557-F1-model_v2	2.339817524	58	P	D
## 796	AF-P35557-F1-model_v2	2.115411997	58	P	E
## 797	AF-P35557-F1-model_v2	1.797528505	58	P	A
## 798	AF-P35557-F1-model_v2	0.915750146	58	P	C
## 799	AF-P35557-F1-model_v2	2.037068129	59	T	A
## 800	AF-P35557-F1-model_v2	1.390208244	59	T	C
## 801	AF-P35557-F1-model_v2	1.639879465	59	T	D
## 802	AF-P35557-F1-model_v2	2.103356123	59	T	E
## 803	AF-P35557-F1-model_v2	1.801752567	59	T	F
## 804	AF-P35557-F1-model_v2	1.982607603	59	T	G
## 805	AF-P35557-F1-model_v2	2.080371618	59	T	H
## 806	AF-P35557-F1-model_v2	2.367770672	59	T	K
## 807	AF-P35557-F1-model_v2	1.646192312	59	T	L
## 808	AF-P35557-F1-model_v2	1.678770542	59	T	M
## 809	AF-P35557-F1-model_v2	2.774865866	59	T	P
## 810	AF-P35557-F1-model_v2	2.020287514	59	T	Q
## 811	AF-P35557-F1-model_v2	2.295866013	59	T	R
## 812	AF-P35557-F1-model_v2	0.727186680	59	T	S

## 813	AF-P35557-F1-model_v2	1.908382058	59	T	V
## 814	AF-P35557-F1-model_v2	1.946656108	59	T	W
## 815	AF-P35557-F1-model_v2	2.000513554	59	T	Y
## 816	AF-P35557-F1-model_v2	1.798502564	60	Y	A
## 817	AF-P35557-F1-model_v2	0.736901283	60	Y	C
## 818	AF-P35557-F1-model_v2	2.373437166	60	Y	D
## 819	AF-P35557-F1-model_v2	2.200634956	60	Y	E
## 820	AF-P35557-F1-model_v2	0.136624455	60	Y	F
## 821	AF-P35557-F1-model_v2	1.402205706	60	Y	G
## 822	AF-P35557-F1-model_v2	0.806076050	60	Y	H
## 823	AF-P35557-F1-model_v2	1.623431563	60	Y	I
## 824	AF-P35557-F1-model_v2	1.623625040	60	Y	K
## 825	AF-P35557-F1-model_v2	1.177243471	60	Y	L
## 826	AF-P35557-F1-model_v2	1.310767412	60	Y	M
## 827	AF-P35557-F1-model_v2	1.728800654	60	Y	N
## 828	AF-P35557-F1-model_v2	1.935613751	60	Y	P
## 829	AF-P35557-F1-model_v2	1.755542874	60	Y	Q
## 830	AF-P35557-F1-model_v2	1.553813100	60	Y	R
## 831	AF-P35557-F1-model_v2	2.044143438	60	Y	S
## 832	AF-P35557-F1-model_v2	2.019083023	60	Y	T
## 833	AF-P35557-F1-model_v2	1.849037170	60	Y	V
## 834	AF-P35557-F1-model_v2	0.842410684	60	Y	W
## 835	AF-P35557-F1-model_v2	1.748289108	61	V	A
## 836	AF-P35557-F1-model_v2	0.870405793	61	V	C
## 837	AF-P35557-F1-model_v2	2.376390696	61	V	E
## 838	AF-P35557-F1-model_v2	1.277887583	61	V	F
## 839	AF-P35557-F1-model_v2	2.251621246	61	V	G
## 840	AF-P35557-F1-model_v2	2.023339272	61	V	H
## 841	AF-P35557-F1-model_v2	-0.137223482	61	V	I
## 842	AF-P35557-F1-model_v2	2.304397583	61	V	K
## 843	AF-P35557-F1-model_v2	0.537673354	61	V	L
## 844	AF-P35557-F1-model_v2	1.091713428	61	V	M
## 845	AF-P35557-F1-model_v2	2.054235220	61	V	N
## 846	AF-P35557-F1-model_v2	2.141302109	61	V	P
## 847	AF-P35557-F1-model_v2	2.221114397	61	V	Q
## 848	AF-P35557-F1-model_v2	2.387529850	61	V	R
## 849	AF-P35557-F1-model_v2	2.078018904	61	V	S
## 850	AF-P35557-F1-model_v2	1.785474062	61	V	T
## 851	AF-P35557-F1-model_v2	1.473268747	61	V	W
## 852	AF-P35557-F1-model_v2	1.570358276	61	V	Y
## 853	AF-P35557-F1-model_v2	-0.061830938	62	R	A
## 854	AF-P35557-F1-model_v2	-0.480378687	62	R	C
## 855	AF-P35557-F1-model_v2	0.226209760	62	R	E
## 856	AF-P35557-F1-model_v2	0.128447592	62	R	F
## 857	AF-P35557-F1-model_v2	0.406719089	62	R	G
## 858	AF-P35557-F1-model_v2	-0.027437627	62	R	D
## 859	AF-P35557-F1-model_v2	-0.088973224	62	R	N
## 860	AF-P35557-F1-model_v2	1.287593603	62	R	P
## 861	AF-P35557-F1-model_v2	0.154431462	62	R	Q
## 862	AF-P35557-F1-model_v2	-0.038055241	62	R	S
## 863	AF-P35557-F1-model_v2	-0.419354379	62	R	T
## 864	AF-P35557-F1-model_v2	-0.236197352	62	R	V
## 865	AF-P35557-F1-model_v2	0.447908521	62	R	W
## 866	AF-P35557-F1-model_v2	0.186410248	62	R	Y

## 867	AF-P35557-F1-model_v2	-0.092928946	62	R	H
## 868	AF-P35557-F1-model_v2	0.039259136	62	R	I
## 869	AF-P35557-F1-model_v2	0.258619279	62	R	K
## 870	AF-P35557-F1-model_v2	-0.107924581	62	R	L
## 871	AF-P35557-F1-model_v2	0.029048741	62	R	M
## 872	AF-P35557-F1-model_v2	0.427470148	63	S	A
## 873	AF-P35557-F1-model_v2	0.023791909	63	S	C
## 874	AF-P35557-F1-model_v2	0.655826688	63	S	D
## 875	AF-P35557-F1-model_v2	0.439055681	63	S	F
## 876	AF-P35557-F1-model_v2	1.094928265	63	S	G
## 877	AF-P35557-F1-model_v2	0.627617180	63	S	H
## 878	AF-P35557-F1-model_v2	0.523548901	63	S	I
## 879	AF-P35557-F1-model_v2	1.102952003	63	S	K
## 880	AF-P35557-F1-model_v2	0.854897022	63	S	L
## 881	AF-P35557-F1-model_v2	0.541035771	63	S	M
## 882	AF-P35557-F1-model_v2	0.750632703	63	S	N
## 883	AF-P35557-F1-model_v2	2.997615576	63	S	P
## 884	AF-P35557-F1-model_v2	0.504324198	63	S	Q
## 885	AF-P35557-F1-model_v2	0.984567642	63	S	R
## 886	AF-P35557-F1-model_v2	0.080006957	63	S	T
## 887	AF-P35557-F1-model_v2	0.248106122	63	S	V
## 888	AF-P35557-F1-model_v2	0.154302359	63	S	W
## 889	AF-P35557-F1-model_v2	0.431220174	63	S	Y
## 890	AF-P35557-F1-model_v2	1.163858294	64	T	A
## 891	AF-P35557-F1-model_v2	0.526436508	64	T	C
## 892	AF-P35557-F1-model_v2	1.839132547	64	T	D
## 893	AF-P35557-F1-model_v2	1.577347994	64	T	E
## 894	AF-P35557-F1-model_v2	1.469579220	64	T	G
## 895	AF-P35557-F1-model_v2	1.077135682	64	T	H
## 896	AF-P35557-F1-model_v2	0.670187593	64	T	I
## 897	AF-P35557-F1-model_v2	1.188739896	64	T	K
## 898	AF-P35557-F1-model_v2	0.376399159	64	T	L
## 899	AF-P35557-F1-model_v2	0.743519187	64	T	M
## 900	AF-P35557-F1-model_v2	1.204722047	64	T	N
## 901	AF-P35557-F1-model_v2	1.289452195	64	T	P
## 902	AF-P35557-F1-model_v2	1.335433483	64	T	Q
## 903	AF-P35557-F1-model_v2	1.206768513	64	T	R
## 904	AF-P35557-F1-model_v2	0.855081499	64	T	S
## 905	AF-P35557-F1-model_v2	0.640085936	64	T	V
## 906	AF-P35557-F1-model_v2	0.660510600	64	T	W
## 907	AF-P35557-F1-model_v2	0.263670564	64	T	Y
## 908	AF-P35557-F1-model_v2	-0.037046909	65	P	I
## 909	AF-P35557-F1-model_v2	0.017431259	65	P	F
## 910	AF-P35557-F1-model_v2	0.721009314	65	P	D
## 911	AF-P35557-F1-model_v2	0.782986343	65	P	K
## 912	AF-P35557-F1-model_v2	0.503012776	65	P	G
## 913	AF-P35557-F1-model_v2	0.601598024	65	P	H
## 914	AF-P35557-F1-model_v2	0.158558965	65	P	V
## 915	AF-P35557-F1-model_v2	0.818573236	65	P	E
## 916	AF-P35557-F1-model_v2	0.506305099	65	P	S
## 917	AF-P35557-F1-model_v2	0.569454312	65	P	T
## 918	AF-P35557-F1-model_v2	0.097583890	65	P	L
## 919	AF-P35557-F1-model_v2	-0.273758590	65	P	W
## 920	AF-P35557-F1-model_v2	0.039847314	65	P	Y

## 921	AF-P35557-F1-model_v2	-0.116751730	65	P	C
## 922	AF-P35557-F1-model_v2	0.654567122	65	P	Q
## 923	AF-P35557-F1-model_v2	0.810426831	65	P	R
## 924	AF-P35557-F1-model_v2	0.195986152	65	P	A
## 925	AF-P35557-F1-model_v2	0.015240431	65	P	M
## 926	AF-P35557-F1-model_v2	0.569582462	66	E	V
## 927	AF-P35557-F1-model_v2	0.681988657	66	E	W
## 928	AF-P35557-F1-model_v2	-0.177953601	66	E	T
## 929	AF-P35557-F1-model_v2	0.209134221	66	E	Q
## 930	AF-P35557-F1-model_v2	0.423638105	66	E	G
## 931	AF-P35557-F1-model_v2	0.327350616	66	E	A
## 932	AF-P35557-F1-model_v2	-0.121962309	66	E	S
## 933	AF-P35557-F1-model_v2	1.175604939	66	E	P
## 934	AF-P35557-F1-model_v2	0.434981287	66	E	H
## 935	AF-P35557-F1-model_v2	0.515481353	66	E	L
## 936	AF-P35557-F1-model_v2	0.881464005	66	E	Y
## 937	AF-P35557-F1-model_v2	0.741499424	66	E	F
## 938	AF-P35557-F1-model_v2	0.117755413	66	E	N
## 939	AF-P35557-F1-model_v2	0.638280034	66	E	I
## 940	AF-P35557-F1-model_v2	0.703069985	66	E	R
## 941	AF-P35557-F1-model_v2	0.474129140	66	E	M
## 942	AF-P35557-F1-model_v2	0.631718993	66	E	K
## 943	AF-P35557-F1-model_v2	-0.357187986	66	E	D
## 944	AF-P35557-F1-model_v2	0.056011736	66	E	C
## 945	AF-P35557-F1-model_v2	0.930772066	67	G	N
## 946	AF-P35557-F1-model_v2	1.132644415	67	G	Q
## 947	AF-P35557-F1-model_v2	2.619082689	67	G	P
## 948	AF-P35557-F1-model_v2	1.647659898	67	G	S
## 949	AF-P35557-F1-model_v2	2.014205217	67	G	I
## 950	AF-P35557-F1-model_v2	0.967843175	67	G	H
## 951	AF-P35557-F1-model_v2	1.421035290	67	G	R
## 952	AF-P35557-F1-model_v2	1.442119122	67	G	W
## 953	AF-P35557-F1-model_v2	1.254267931	67	G	K
## 954	AF-P35557-F1-model_v2	2.050164700	67	G	T
## 955	AF-P35557-F1-model_v2	2.055108786	67	G	V
## 956	AF-P35557-F1-model_v2	1.255061626	67	G	Y
## 957	AF-P35557-F1-model_v2	0.961013734	67	G	M
## 958	AF-P35557-F1-model_v2	1.110084057	67	G	L
## 959	AF-P35557-F1-model_v2	0.991685033	67	G	F
## 960	AF-P35557-F1-model_v2	0.554610848	67	G	C
## 961	AF-P35557-F1-model_v2	1.536290526	67	G	A
## 962	AF-P35557-F1-model_v2	1.522239447	67	G	E
## 963	AF-P35557-F1-model_v2	0.431929111	68	S	A
## 964	AF-P35557-F1-model_v2	0.162580848	68	S	C
## 965	AF-P35557-F1-model_v2	0.416959882	68	S	D
## 966	AF-P35557-F1-model_v2	0.604245365	68	S	E
## 967	AF-P35557-F1-model_v2	0.631252348	68	S	F
## 968	AF-P35557-F1-model_v2	0.403304338	68	S	G
## 969	AF-P35557-F1-model_v2	0.322701275	68	S	H
## 970	AF-P35557-F1-model_v2	0.811035872	68	S	I
## 971	AF-P35557-F1-model_v2	0.421889007	68	S	K
## 972	AF-P35557-F1-model_v2	0.681563735	68	S	L
## 973	AF-P35557-F1-model_v2	0.593723834	68	S	M
## 974	AF-P35557-F1-model_v2	-0.009671569	68	S	N

## 975	AF-P35557-F1-model_v2	1.687964797	68	S	P
## 976	AF-P35557-F1-model_v2	0.384684682	68	S	Q
## 977	AF-P35557-F1-model_v2	0.418558598	68	S	R
## 978	AF-P35557-F1-model_v2	0.062978387	68	S	T
## 979	AF-P35557-F1-model_v2	0.642218590	68	S	V
## 980	AF-P35557-F1-model_v2	0.683870733	68	S	W
## 981	AF-P35557-F1-model_v2	0.648389995	68	S	Y
## 982	AF-P35557-F1-model_v2	1.480406761	69	E	W
## 983	AF-P35557-F1-model_v2	1.361429214	69	E	F
## 984	AF-P35557-F1-model_v2	1.528334618	69	E	S
## 985	AF-P35557-F1-model_v2	1.402370572	69	E	G
## 986	AF-P35557-F1-model_v2	1.279269457	69	E	T
## 987	AF-P35557-F1-model_v2	1.709576726	69	E	V
## 988	AF-P35557-F1-model_v2	1.055807948	69	E	Y
## 989	AF-P35557-F1-model_v2	1.134770989	69	E	C
## 990	AF-P35557-F1-model_v2	1.101641655	69	E	H
## 991	AF-P35557-F1-model_v2	1.320271134	69	E	A
## 992	AF-P35557-F1-model_v2	1.769124031	69	E	R
## 993	AF-P35557-F1-model_v2	0.610602975	69	E	Q
## 994	AF-P35557-F1-model_v2	1.086478829	69	E	M
## 995	AF-P35557-F1-model_v2	1.550422907	69	E	L
## 996	AF-P35557-F1-model_v2	1.527320147	69	E	I
## 997	AF-P35557-F1-model_v2	1.419659257	69	E	P
## 998	AF-P35557-F1-model_v2	1.557633638	69	E	N
## 999	AF-P35557-F1-model_v2	1.777036786	69	E	K
## 1000	AF-P35557-F1-model_v2	0.073199809	70	V	A
## 1001	AF-P35557-F1-model_v2	-0.120596707	70	V	C
## 1002	AF-P35557-F1-model_v2	0.768203020	70	V	D
## 1003	AF-P35557-F1-model_v2	0.643411756	70	V	E
## 1004	AF-P35557-F1-model_v2	0.251593888	70	V	F
## 1005	AF-P35557-F1-model_v2	0.378578842	70	V	G
## 1006	AF-P35557-F1-model_v2	-0.041423261	70	V	H
## 1007	AF-P35557-F1-model_v2	-0.234374583	70	V	K
## 1008	AF-P35557-F1-model_v2	0.114100933	70	V	L
## 1009	AF-P35557-F1-model_v2	0.135514379	70	V	M
## 1010	AF-P35557-F1-model_v2	0.085183203	70	V	N
## 1011	AF-P35557-F1-model_v2	0.758971691	70	V	P
## 1012	AF-P35557-F1-model_v2	0.088813066	70	V	Q
## 1013	AF-P35557-F1-model_v2	-0.234065711	70	V	R
## 1014	AF-P35557-F1-model_v2	0.050828338	70	V	S
## 1015	AF-P35557-F1-model_v2	0.078463614	70	V	T
## 1016	AF-P35557-F1-model_v2	0.557821393	70	V	W
## 1017	AF-P35557-F1-model_v2	0.298563063	70	V	Y
## 1018	AF-P35557-F1-model_v2	1.804981709	71	G	M
## 1019	AF-P35557-F1-model_v2	2.387250662	71	G	T
## 1020	AF-P35557-F1-model_v2	1.855836868	71	G	V
## 1021	AF-P35557-F1-model_v2	2.334626436	71	G	Q
## 1022	AF-P35557-F1-model_v2	1.923570514	71	G	L
## 1023	AF-P35557-F1-model_v2	2.206399679	71	G	S
## 1024	AF-P35557-F1-model_v2	2.501935482	71	G	P
## 1025	AF-P35557-F1-model_v2	1.804329872	71	G	A
## 1026	AF-P35557-F1-model_v2	1.796950102	71	G	W
## 1027	AF-P35557-F1-model_v2	2.420535564	71	G	N
## 1028	AF-P35557-F1-model_v2	1.800082922	71	G	Y

## 1029	AF-P35557-F1-model_v2	2.591179371	71	G	E
## 1030	AF-P35557-F1-model_v2	2.006510735	71	G	I
## 1031	AF-P35557-F1-model_v2	2.419834614	71	G	R
## 1032	AF-P35557-F1-model_v2	1.566017985	71	G	F
## 1033	AF-P35557-F1-model_v2	2.524516106	71	G	K
## 1034	AF-P35557-F1-model_v2	2.592098951	71	G	D
## 1035	AF-P35557-F1-model_v2	2.187266827	71	G	H
## 1036	AF-P35557-F1-model_v2	0.989345312	72	D	V
## 1037	AF-P35557-F1-model_v2	0.835007071	72	D	S
## 1038	AF-P35557-F1-model_v2	0.864196777	72	D	T
## 1039	AF-P35557-F1-model_v2	0.620664060	72	D	C
## 1040	AF-P35557-F1-model_v2	1.178735614	72	D	A
## 1041	AF-P35557-F1-model_v2	0.847185016	72	D	F
## 1042	AF-P35557-F1-model_v2	1.072241783	72	D	Y
## 1043	AF-P35557-F1-model_v2	1.902121186	72	D	G
## 1044	AF-P35557-F1-model_v2	1.359070182	72	D	H
## 1045	AF-P35557-F1-model_v2	0.334950328	72	D	E
## 1046	AF-P35557-F1-model_v2	1.789913654	72	D	K
## 1047	AF-P35557-F1-model_v2	1.866785169	72	D	R
## 1048	AF-P35557-F1-model_v2	0.804444253	72	D	I
## 1049	AF-P35557-F1-model_v2	0.467114329	72	D	W
## 1050	AF-P35557-F1-model_v2	0.878117800	72	D	M
## 1051	AF-P35557-F1-model_v2	0.803319812	72	D	Q
## 1052	AF-P35557-F1-model_v2	1.134065509	72	D	N
## 1053	AF-P35557-F1-model_v2	0.906800449	72	D	L
## 1054	AF-P35557-F1-model_v2	1.942644715	72	D	P
## 1055	AF-P35557-F1-model_v2	3.136154175	73	F	D
## 1056	AF-P35557-F1-model_v2	0.814507365	73	F	Y
## 1057	AF-P35557-F1-model_v2	2.391463280	73	F	H
## 1058	AF-P35557-F1-model_v2	1.865276814	73	F	V
## 1059	AF-P35557-F1-model_v2	2.849694252	73	F	G
## 1060	AF-P35557-F1-model_v2	2.782670975	73	F	S
## 1061	AF-P35557-F1-model_v2	2.721524239	73	F	A
## 1062	AF-P35557-F1-model_v2	2.797625780	73	F	E
## 1063	AF-P35557-F1-model_v2	2.589690685	73	F	T
## 1064	AF-P35557-F1-model_v2	2.738151073	73	F	Q
## 1065	AF-P35557-F1-model_v2	2.486587763	73	F	R
## 1066	AF-P35557-F1-model_v2	2.878822327	73	F	N
## 1067	AF-P35557-F1-model_v2	1.747845411	73	F	C
## 1068	AF-P35557-F1-model_v2	2.530787230	73	F	P
## 1069	AF-P35557-F1-model_v2	1.593368888	73	F	M
## 1070	AF-P35557-F1-model_v2	2.592594862	73	F	K
## 1071	AF-P35557-F1-model_v2	1.189225674	73	F	W
## 1072	AF-P35557-F1-model_v2	1.468311667	73	F	I
## 1073	AF-P35557-F1-model_v2	1.488593936	73	F	L
## 1074	AF-P35557-F1-model_v2	2.706820250	74	L	H
## 1075	AF-P35557-F1-model_v2	0.851306319	74	L	I
## 1076	AF-P35557-F1-model_v2	2.655589342	74	L	E
## 1077	AF-P35557-F1-model_v2	1.061073661	74	L	F
## 1078	AF-P35557-F1-model_v2	2.917033195	74	L	K
## 1079	AF-P35557-F1-model_v2	2.115572929	74	L	A
## 1080	AF-P35557-F1-model_v2	0.674828887	74	L	M
## 1081	AF-P35557-F1-model_v2	2.379774332	74	L	G
## 1082	AF-P35557-F1-model_v2	2.890683174	74	L	D

## 1083	AF-P35557-F1-model_v2	2.587079048	74	L	P
## 1084	AF-P35557-F1-model_v2	2.563133001	74	L	T
## 1085	AF-P35557-F1-model_v2	1.326190829	74	L	V
## 1086	AF-P35557-F1-model_v2	2.782122374	74	L	N
## 1087	AF-P35557-F1-model_v2	1.924947262	74	L	Y
## 1088	AF-P35557-F1-model_v2	1.421531677	74	L	C
## 1089	AF-P35557-F1-model_v2	2.745542526	74	L	Q
## 1090	AF-P35557-F1-model_v2	2.844700575	74	L	R
## 1091	AF-P35557-F1-model_v2	1.920286536	74	L	W
## 1092	AF-P35557-F1-model_v2	2.765895605	74	L	S
## 1093	AF-P35557-F1-model_v2	-0.399899840	75	S	A
## 1094	AF-P35557-F1-model_v2	0.177937269	75	S	C
## 1095	AF-P35557-F1-model_v2	1.988531947	75	S	D
## 1096	AF-P35557-F1-model_v2	1.592318535	75	S	E
## 1097	AF-P35557-F1-model_v2	0.748253584	75	S	F
## 1098	AF-P35557-F1-model_v2	0.635037422	75	S	G
## 1099	AF-P35557-F1-model_v2	1.775323868	75	S	H
## 1100	AF-P35557-F1-model_v2	1.724984646	75	S	K
## 1101	AF-P35557-F1-model_v2	1.344612837	75	S	L
## 1102	AF-P35557-F1-model_v2	0.889805675	75	S	M
## 1103	AF-P35557-F1-model_v2	1.953159928	75	S	N
## 1104	AF-P35557-F1-model_v2	1.586459160	75	S	P
## 1105	AF-P35557-F1-model_v2	1.569252133	75	S	Q
## 1106	AF-P35557-F1-model_v2	1.626341105	75	S	R
## 1107	AF-P35557-F1-model_v2	0.431362748	75	S	T
## 1108	AF-P35557-F1-model_v2	0.321543336	75	S	V
## 1109	AF-P35557-F1-model_v2	0.858639956	75	S	W
## 1110	AF-P35557-F1-model_v2	1.182523131	75	S	Y
## 1111	AF-P35557-F1-model_v2	2.915218830	76	L	D
## 1112	AF-P35557-F1-model_v2	1.141358376	76	L	F
## 1113	AF-P35557-F1-model_v2	2.172397375	76	L	G
## 1114	AF-P35557-F1-model_v2	0.756442070	76	L	C
## 1115	AF-P35557-F1-model_v2	2.284583330	76	L	H
## 1116	AF-P35557-F1-model_v2	2.512901783	76	L	E
## 1117	AF-P35557-F1-model_v2	2.134291410	76	L	S
## 1118	AF-P35557-F1-model_v2	1.728370190	76	L	T
## 1119	AF-P35557-F1-model_v2	2.828297615	76	L	P
## 1120	AF-P35557-F1-model_v2	2.385812521	76	L	Q
## 1121	AF-P35557-F1-model_v2	2.336414337	76	L	R
## 1122	AF-P35557-F1-model_v2	1.517647505	76	L	A
## 1123	AF-P35557-F1-model_v2	2.454304695	76	L	N
## 1124	AF-P35557-F1-model_v2	0.477359056	76	L	V
## 1125	AF-P35557-F1-model_v2	1.516445041	76	L	W
## 1126	AF-P35557-F1-model_v2	1.502386570	76	L	Y
## 1127	AF-P35557-F1-model_v2	0.768509388	76	L	M
## 1128	AF-P35557-F1-model_v2	0.083450317	76	L	I
## 1129	AF-P35557-F1-model_v2	2.271793604	76	L	K
## 1130	AF-P35557-F1-model_v2	2.086027622	85	V	A
## 1131	AF-P35557-F1-model_v2	1.280158162	85	V	C
## 1132	AF-P35557-F1-model_v2	3.034178495	85	V	D
## 1133	AF-P35557-F1-model_v2	3.075663805	85	V	E
## 1134	AF-P35557-F1-model_v2	1.800702572	85	V	F
## 1135	AF-P35557-F1-model_v2	2.714928865	85	V	G
## 1136	AF-P35557-F1-model_v2	2.816030264	85	V	H

## 1137	AF-P35557-F1-model_v2	0.456487417	85	V	I
## 1138	AF-P35557-F1-model_v2	2.979702950	85	V	K
## 1139	AF-P35557-F1-model_v2	1.329364657	85	V	L
## 1140	AF-P35557-F1-model_v2	1.990046263	85	V	M
## 1141	AF-P35557-F1-model_v2	2.987277269	85	V	N
## 1142	AF-P35557-F1-model_v2	2.480928898	85	V	P
## 1143	AF-P35557-F1-model_v2	3.094729424	85	V	Q
## 1144	AF-P35557-F1-model_v2	3.023630142	85	V	R
## 1145	AF-P35557-F1-model_v2	2.862968206	85	V	S
## 1146	AF-P35557-F1-model_v2	2.168448925	85	V	T
## 1147	AF-P35557-F1-model_v2	2.249892473	85	V	W
## 1148	AF-P35557-F1-model_v2	2.177119255	85	V	Y
## 1149	AF-P35557-F1-model_v2	0.216077805	86	M	Y
## 1150	AF-P35557-F1-model_v2	0.296236634	86	M	V
## 1151	AF-P35557-F1-model_v2	0.214001775	86	M	W
## 1152	AF-P35557-F1-model_v2	0.823377013	86	M	A
## 1153	AF-P35557-F1-model_v2	0.288314939	86	M	C
## 1154	AF-P35557-F1-model_v2	1.739907384	86	M	D
## 1155	AF-P35557-F1-model_v2	1.352845073	86	M	E
## 1156	AF-P35557-F1-model_v2	-0.371567011	86	M	F
## 1157	AF-P35557-F1-model_v2	1.788398623	86	M	R
## 1158	AF-P35557-F1-model_v2	1.177080393	86	M	S
## 1159	AF-P35557-F1-model_v2	1.126015425	86	M	T
## 1160	AF-P35557-F1-model_v2	0.314400554	86	M	I
## 1161	AF-P35557-F1-model_v2	1.330772400	86	M	Q
## 1162	AF-P35557-F1-model_v2	1.944456816	86	M	G
## 1163	AF-P35557-F1-model_v2	1.062058449	86	M	H
## 1164	AF-P35557-F1-model_v2	2.049609900	86	M	P
## 1165	AF-P35557-F1-model_v2	1.528653741	86	M	N
## 1166	AF-P35557-F1-model_v2	0.310951829	86	M	L
## 1167	AF-P35557-F1-model_v2	2.535757542	87	L	K
## 1168	AF-P35557-F1-model_v2	3.200241327	87	L	G
## 1169	AF-P35557-F1-model_v2	0.631908894	87	L	I
## 1170	AF-P35557-F1-model_v2	2.861814976	87	L	E
## 1171	AF-P35557-F1-model_v2	1.003126264	87	L	F
## 1172	AF-P35557-F1-model_v2	2.347676754	87	L	H
## 1173	AF-P35557-F1-model_v2	3.380879164	87	L	D
## 1174	AF-P35557-F1-model_v2	2.542724848	87	L	T
## 1175	AF-P35557-F1-model_v2	1.353615522	87	L	V
## 1176	AF-P35557-F1-model_v2	1.297957897	87	L	Y
## 1177	AF-P35557-F1-model_v2	2.337860346	87	L	A
## 1178	AF-P35557-F1-model_v2	1.337089658	87	L	C
## 1179	AF-P35557-F1-model_v2	0.944157124	87	L	M
## 1180	AF-P35557-F1-model_v2	1.279874563	87	L	W
## 1181	AF-P35557-F1-model_v2	3.223864079	87	L	P
## 1182	AF-P35557-F1-model_v2	2.836917400	87	L	S
## 1183	AF-P35557-F1-model_v2	2.540787935	87	L	R
## 1184	AF-P35557-F1-model_v2	3.137443066	87	L	N
## 1185	AF-P35557-F1-model_v2	2.288629055	88	V	A
## 1186	AF-P35557-F1-model_v2	1.344813466	88	V	C
## 1187	AF-P35557-F1-model_v2	2.910982132	88	V	E
## 1188	AF-P35557-F1-model_v2	1.449757576	88	V	F
## 1189	AF-P35557-F1-model_v2	3.396425247	88	V	G
## 1190	AF-P35557-F1-model_v2	2.411315441	88	V	H

## 1191	AF-P35557-F1-model_v2	0.223042727	88	V	I
## 1192	AF-P35557-F1-model_v2	2.923849821	88	V	K
## 1193	AF-P35557-F1-model_v2	1.401281714	88	V	L
## 1194	AF-P35557-F1-model_v2	1.707838655	88	V	M
## 1195	AF-P35557-F1-model_v2	2.934157610	88	V	N
## 1196	AF-P35557-F1-model_v2	3.337833405	88	V	P
## 1197	AF-P35557-F1-model_v2	2.678389549	88	V	Q
## 1198	AF-P35557-F1-model_v2	2.954785109	88	V	R
## 1199	AF-P35557-F1-model_v2	2.861024857	88	V	S
## 1200	AF-P35557-F1-model_v2	2.142478943	88	V	T
## 1201	AF-P35557-F1-model_v2	1.805590630	88	V	W
## 1202	AF-P35557-F1-model_v2	1.694304943	88	V	Y
## 1203	AF-P35557-F1-model_v2	0.358447671	89	K	E
## 1204	AF-P35557-F1-model_v2	-0.275006950	89	K	C
## 1205	AF-P35557-F1-model_v2	-0.079783142	89	K	H
## 1206	AF-P35557-F1-model_v2	-0.133723319	89	K	Y
## 1207	AF-P35557-F1-model_v2	1.258194089	89	K	G
## 1208	AF-P35557-F1-model_v2	0.301531672	89	K	N
## 1209	AF-P35557-F1-model_v2	-0.043400109	89	K	F
## 1210	AF-P35557-F1-model_v2	0.751554072	89	K	D
## 1211	AF-P35557-F1-model_v2	0.013744473	89	K	W
## 1212	AF-P35557-F1-model_v2	-0.287599981	89	K	T
## 1213	AF-P35557-F1-model_v2	-0.017812073	89	K	R
## 1214	AF-P35557-F1-model_v2	-0.371246159	89	K	V
## 1215	AF-P35557-F1-model_v2	0.106689095	89	K	L
## 1216	AF-P35557-F1-model_v2	0.067682505	89	K	M
## 1217	AF-P35557-F1-model_v2	0.008130074	89	K	Q
## 1218	AF-P35557-F1-model_v2	-0.349973381	89	K	I
## 1219	AF-P35557-F1-model_v2	0.583348095	89	K	A
## 1220	AF-P35557-F1-model_v2	0.108524859	89	K	S
## 1221	AF-P35557-F1-model_v2	2.061636925	89	K	P
## 1222	AF-P35557-F1-model_v2	2.149024010	90	V	A
## 1223	AF-P35557-F1-model_v2	0.900389910	90	V	C
## 1224	AF-P35557-F1-model_v2	3.144256115	90	V	D
## 1225	AF-P35557-F1-model_v2	2.931322098	90	V	E
## 1226	AF-P35557-F1-model_v2	1.737707615	90	V	F
## 1227	AF-P35557-F1-model_v2	2.826443911	90	V	G
## 1228	AF-P35557-F1-model_v2	2.773629427	90	V	H
## 1229	AF-P35557-F1-model_v2	0.183652878	90	V	I
## 1230	AF-P35557-F1-model_v2	2.897808790	90	V	K
## 1231	AF-P35557-F1-model_v2	1.103393197	90	V	L
## 1232	AF-P35557-F1-model_v2	1.586465597	90	V	M
## 1233	AF-P35557-F1-model_v2	2.828697681	90	V	N
## 1234	AF-P35557-F1-model_v2	2.767657042	90	V	P
## 1235	AF-P35557-F1-model_v2	2.823816538	90	V	Q
## 1236	AF-P35557-F1-model_v2	3.105273008	90	V	R
## 1237	AF-P35557-F1-model_v2	2.541355371	90	V	S
## 1238	AF-P35557-F1-model_v2	1.920772314	90	V	T
## 1239	AF-P35557-F1-model_v2	2.405821323	90	V	W
## 1240	AF-P35557-F1-model_v2	2.305397511	90	V	Y
## 1241	AF-P35557-F1-model_v2	0.667869687	91	G	T
## 1242	AF-P35557-F1-model_v2	1.120779753	91	G	D
## 1243	AF-P35557-F1-model_v2	1.127830386	91	G	E
## 1244	AF-P35557-F1-model_v2	1.187965870	91	G	R

## 1245	AF-P35557-F1-model_v2	0.211077452	91	G	C
## 1246	AF-P35557-F1-model_v2	0.834689319	91	G	I
## 1247	AF-P35557-F1-model_v2	0.884126782	91	G	L
## 1248	AF-P35557-F1-model_v2	1.018746376	91	G	Q
## 1249	AF-P35557-F1-model_v2	0.762975752	91	G	H
## 1250	AF-P35557-F1-model_v2	0.384364903	91	G	W
## 1251	AF-P35557-F1-model_v2	0.649631858	91	G	S
## 1252	AF-P35557-F1-model_v2	1.889340401	91	G	P
## 1253	AF-P35557-F1-model_v2	0.110530972	91	G	F
## 1254	AF-P35557-F1-model_v2	0.382346034	91	G	Y
## 1255	AF-P35557-F1-model_v2	0.800364375	91	G	V
## 1256	AF-P35557-F1-model_v2	0.994998455	91	G	N
## 1257	AF-P35557-F1-model_v2	0.753675699	91	G	M
## 1258	AF-P35557-F1-model_v2	0.913723230	91	G	A
## 1259	AF-P35557-F1-model_v2	-0.482845128	92	E	W
## 1260	AF-P35557-F1-model_v2	0.524797559	92	E	D
## 1261	AF-P35557-F1-model_v2	-0.530182481	92	E	V
## 1262	AF-P35557-F1-model_v2	-0.615532994	92	E	L
## 1263	AF-P35557-F1-model_v2	-0.154125810	92	E	H
## 1264	AF-P35557-F1-model_v2	-0.463686168	92	E	Y
## 1265	AF-P35557-F1-model_v2	-0.300306976	92	E	K
## 1266	AF-P35557-F1-model_v2	0.582491040	92	E	G
## 1267	AF-P35557-F1-model_v2	0.118054152	92	E	S
## 1268	AF-P35557-F1-model_v2	-0.486221015	92	E	F
## 1269	AF-P35557-F1-model_v2	-0.217415214	92	E	T
## 1270	AF-P35557-F1-model_v2	0.089569330	92	E	A
## 1271	AF-P35557-F1-model_v2	-0.305256546	92	E	R
## 1272	AF-P35557-F1-model_v2	-0.440838635	92	E	M
## 1273	AF-P35557-F1-model_v2	-0.650608897	92	E	I
## 1274	AF-P35557-F1-model_v2	-0.463862300	92	E	C
## 1275	AF-P35557-F1-model_v2	0.212900251	92	E	N
## 1276	AF-P35557-F1-model_v2	-0.106956542	92	E	Q
## 1277	AF-P35557-F1-model_v2	-0.472871006	92	E	P
## 1278	AF-P35557-F1-model_v2	0.832318723	93	G	C
## 1279	AF-P35557-F1-model_v2	1.145337820	93	G	Y
## 1280	AF-P35557-F1-model_v2	1.156824708	93	G	W
## 1281	AF-P35557-F1-model_v2	1.023428082	93	G	F
## 1282	AF-P35557-F1-model_v2	1.010561228	93	G	I
## 1283	AF-P35557-F1-model_v2	1.516479015	93	G	K
## 1284	AF-P35557-F1-model_v2	0.995267749	93	G	V
## 1285	AF-P35557-F1-model_v2	1.616296887	93	G	D
## 1286	AF-P35557-F1-model_v2	1.727316737	93	G	E
## 1287	AF-P35557-F1-model_v2	1.198058844	93	G	M
## 1288	AF-P35557-F1-model_v2	1.209524632	93	G	T
## 1289	AF-P35557-F1-model_v2	1.125996590	93	G	A
## 1290	AF-P35557-F1-model_v2	1.080187321	93	G	L
## 1291	AF-P35557-F1-model_v2	1.632238150	93	G	P
## 1292	AF-P35557-F1-model_v2	1.514202476	93	G	R
## 1293	AF-P35557-F1-model_v2	1.204578161	93	G	S
## 1294	AF-P35557-F1-model_v2	1.552610517	93	G	Q
## 1295	AF-P35557-F1-model_v2	1.473158121	93	G	N
## 1296	AF-P35557-F1-model_v2	0.384618223	94	E	K
## 1297	AF-P35557-F1-model_v2	0.462668598	94	E	Y
## 1298	AF-P35557-F1-model_v2	0.310658216	94	E	D

## 1299	AF-P35557-F1-model_v2	0.130028009	94	E	A
## 1300	AF-P35557-F1-model_v2	0.428346336	94	E	F
## 1301	AF-P35557-F1-model_v2	0.366596639	94	E	I
## 1302	AF-P35557-F1-model_v2	0.272943795	94	E	H
## 1303	AF-P35557-F1-model_v2	0.404611766	94	E	L
## 1304	AF-P35557-F1-model_v2	0.518334627	94	E	W
## 1305	AF-P35557-F1-model_v2	0.313244164	94	E	T
## 1306	AF-P35557-F1-model_v2	0.126770675	94	E	C
## 1307	AF-P35557-F1-model_v2	0.335677743	94	E	M
## 1308	AF-P35557-F1-model_v2	0.417108357	94	E	N
## 1309	AF-P35557-F1-model_v2	0.450613916	94	E	G
## 1310	AF-P35557-F1-model_v2	0.488933921	94	E	R
## 1311	AF-P35557-F1-model_v2	0.151499450	94	E	S
## 1312	AF-P35557-F1-model_v2	0.129176915	94	E	Q
## 1313	AF-P35557-F1-model_v2	0.397411644	94	E	V
## 1314	AF-P35557-F1-model_v2	-0.050668716	94	E	P
## 1315	AF-P35557-F1-model_v2	-0.256425858	95	E	Y
## 1316	AF-P35557-F1-model_v2	-0.536706567	95	E	C
## 1317	AF-P35557-F1-model_v2	0.838752866	95	E	P
## 1318	AF-P35557-F1-model_v2	0.322981983	95	E	I
## 1319	AF-P35557-F1-model_v2	-0.264617860	95	E	H
## 1320	AF-P35557-F1-model_v2	-0.175723672	95	E	L
## 1321	AF-P35557-F1-model_v2	-0.110477567	95	E	D
## 1322	AF-P35557-F1-model_v2	-0.040839672	95	E	A
## 1323	AF-P35557-F1-model_v2	-0.282755017	95	E	W
## 1324	AF-P35557-F1-model_v2	-0.351967335	95	E	F
## 1325	AF-P35557-F1-model_v2	-0.201987386	95	E	G
## 1326	AF-P35557-F1-model_v2	-0.095608711	95	E	K
## 1327	AF-P35557-F1-model_v2	-0.405041099	95	E	N
## 1328	AF-P35557-F1-model_v2	0.084728420	95	E	T
## 1329	AF-P35557-F1-model_v2	-0.074028611	95	E	S
## 1330	AF-P35557-F1-model_v2	-0.064599335	95	E	Q
## 1331	AF-P35557-F1-model_v2	0.344816566	95	E	V
## 1332	AF-P35557-F1-model_v2	-0.052232385	95	E	R
## 1333	AF-P35557-F1-model_v2	-0.152936161	95	E	M
## 1334	AF-P35557-F1-model_v2	0.645442128	96	G	C
## 1335	AF-P35557-F1-model_v2	1.657601237	96	G	D
## 1336	AF-P35557-F1-model_v2	1.299986601	96	G	L
## 1337	AF-P35557-F1-model_v2	1.330269337	96	G	A
## 1338	AF-P35557-F1-model_v2	2.233616114	96	G	P
## 1339	AF-P35557-F1-model_v2	1.136755943	96	G	K
## 1340	AF-P35557-F1-model_v2	1.139693975	96	G	R
## 1341	AF-P35557-F1-model_v2	1.676931858	96	G	E
## 1342	AF-P35557-F1-model_v2	0.911073685	96	G	N
## 1343	AF-P35557-F1-model_v2	1.244149923	96	G	Q
## 1344	AF-P35557-F1-model_v2	1.256909847	96	G	Y
## 1345	AF-P35557-F1-model_v2	1.428222895	96	G	W
## 1346	AF-P35557-F1-model_v2	1.417147160	96	G	S
## 1347	AF-P35557-F1-model_v2	1.977670789	96	G	I
## 1348	AF-P35557-F1-model_v2	0.880911589	96	G	H
## 1349	AF-P35557-F1-model_v2	1.838002086	96	G	T
## 1350	AF-P35557-F1-model_v2	1.115801454	96	G	F
## 1351	AF-P35557-F1-model_v2	1.928533554	96	G	V
## 1352	AF-P35557-F1-model_v2	0.181104720	97	Q	H

## 1353	AF-P35557-F1-model_v2	0.113948464	97	Q	I
## 1354	AF-P35557-F1-model_v2	0.127924919	97	Q	L
## 1355	AF-P35557-F1-model_v2	0.111061156	97	Q	M
## 1356	AF-P35557-F1-model_v2	0.199169695	97	Q	N
## 1357	AF-P35557-F1-model_v2	-0.166034698	97	Q	K
## 1358	AF-P35557-F1-model_v2	0.428720713	97	Q	W
## 1359	AF-P35557-F1-model_v2	0.321409583	97	Q	Y
## 1360	AF-P35557-F1-model_v2	0.606212258	97	Q	G
## 1361	AF-P35557-F1-model_v2	0.147961974	97	Q	T
## 1362	AF-P35557-F1-model_v2	1.884864211	97	Q	P
## 1363	AF-P35557-F1-model_v2	-0.168173790	97	Q	R
## 1364	AF-P35557-F1-model_v2	0.320093036	97	Q	S
## 1365	AF-P35557-F1-model_v2	0.077597380	97	Q	V
## 1366	AF-P35557-F1-model_v2	0.344757199	97	Q	E
## 1367	AF-P35557-F1-model_v2	0.279346466	97	Q	F
## 1368	AF-P35557-F1-model_v2	0.247991800	97	Q	A
## 1369	AF-P35557-F1-model_v2	0.025343060	97	Q	C
## 1370	AF-P35557-F1-model_v2	0.667151749	97	Q	D
## 1371	AF-P35557-F1-model_v2	3.095078945	98	W	A
## 1372	AF-P35557-F1-model_v2	1.781103969	98	W	C
## 1373	AF-P35557-F1-model_v2	3.268577814	98	W	D
## 1374	AF-P35557-F1-model_v2	3.282589197	98	W	E
## 1375	AF-P35557-F1-model_v2	0.909697294	98	W	F
## 1376	AF-P35557-F1-model_v2	3.174492359	98	W	G
## 1377	AF-P35557-F1-model_v2	2.418914557	98	W	H
## 1378	AF-P35557-F1-model_v2	2.305943966	98	W	I
## 1379	AF-P35557-F1-model_v2	2.344048023	98	W	K
## 1380	AF-P35557-F1-model_v2	2.078635216	98	W	L
## 1381	AF-P35557-F1-model_v2	1.879399061	98	W	M
## 1382	AF-P35557-F1-model_v2	3.056749821	98	W	N
## 1383	AF-P35557-F1-model_v2	2.398868084	98	W	P
## 1384	AF-P35557-F1-model_v2	2.775155306	98	W	Q
## 1385	AF-P35557-F1-model_v2	2.071568489	98	W	R
## 1386	AF-P35557-F1-model_v2	2.945124865	98	W	S
## 1387	AF-P35557-F1-model_v2	2.947589397	98	W	T
## 1388	AF-P35557-F1-model_v2	2.522757530	98	W	V
## 1389	AF-P35557-F1-model_v2	0.947257161	98	W	Y
## 1390	AF-P35557-F1-model_v2	0.230279505	99	S	A
## 1391	AF-P35557-F1-model_v2	-0.378532231	99	S	C
## 1392	AF-P35557-F1-model_v2	1.231119633	99	S	D
## 1393	AF-P35557-F1-model_v2	0.286515474	99	S	E
## 1394	AF-P35557-F1-model_v2	-0.025324285	99	S	F
## 1395	AF-P35557-F1-model_v2	1.103627563	99	S	G
## 1396	AF-P35557-F1-model_v2	0.303235054	99	S	H
## 1397	AF-P35557-F1-model_v2	0.373539388	99	S	K
## 1398	AF-P35557-F1-model_v2	0.158452690	99	S	L
## 1399	AF-P35557-F1-model_v2	-0.149368823	99	S	M
## 1400	AF-P35557-F1-model_v2	0.824291945	99	S	N
## 1401	AF-P35557-F1-model_v2	2.042084932	99	S	P
## 1402	AF-P35557-F1-model_v2	0.220268905	99	S	Q
## 1403	AF-P35557-F1-model_v2	0.138615847	99	S	R
## 1404	AF-P35557-F1-model_v2	-0.308966100	99	S	T
## 1405	AF-P35557-F1-model_v2	-0.601072490	99	S	V
## 1406	AF-P35557-F1-model_v2	0.113011301	99	S	Y

## 1407	AF-P35557-F1-model_v2	1.735185266	100	V	A
## 1408	AF-P35557-F1-model_v2	0.911659241	100	V	C
## 1409	AF-P35557-F1-model_v2	2.735496044	100	V	D
## 1410	AF-P35557-F1-model_v2	2.557617903	100	V	E
## 1411	AF-P35557-F1-model_v2	1.095641971	100	V	F
## 1412	AF-P35557-F1-model_v2	2.425113440	100	V	G
## 1413	AF-P35557-F1-model_v2	2.375524759	100	V	H
## 1414	AF-P35557-F1-model_v2	-0.071101427	100	V	I
## 1415	AF-P35557-F1-model_v2	2.603760958	100	V	K
## 1416	AF-P35557-F1-model_v2	0.270893693	100	V	L
## 1417	AF-P35557-F1-model_v2	0.900413513	100	V	M
## 1418	AF-P35557-F1-model_v2	2.623231173	100	V	N
## 1419	AF-P35557-F1-model_v2	2.311707735	100	V	P
## 1420	AF-P35557-F1-model_v2	2.515421391	100	V	Q
## 1421	AF-P35557-F1-model_v2	2.595283270	100	V	R
## 1422	AF-P35557-F1-model_v2	2.413597584	100	V	S
## 1423	AF-P35557-F1-model_v2	1.807202816	100	V	T
## 1424	AF-P35557-F1-model_v2	1.494666576	100	V	W
## 1425	AF-P35557-F1-model_v2	1.618991852	100	V	Y
## 1426	AF-P35557-F1-model_v2	-0.231661856	101	K	F
## 1427	AF-P35557-F1-model_v2	0.315279543	101	K	D
## 1428	AF-P35557-F1-model_v2	-0.023089826	101	K	E
## 1429	AF-P35557-F1-model_v2	0.002217412	101	K	S
## 1430	AF-P35557-F1-model_v2	0.996010184	101	K	G
## 1431	AF-P35557-F1-model_v2	-0.368152738	101	K	C
## 1432	AF-P35557-F1-model_v2	0.285664499	101	K	A
## 1433	AF-P35557-F1-model_v2	-0.242375255	101	K	T
## 1434	AF-P35557-F1-model_v2	-0.540281296	101	K	V
## 1435	AF-P35557-F1-model_v2	-0.208123744	101	K	Y
## 1436	AF-P35557-F1-model_v2	-0.036307991	101	K	W
## 1437	AF-P35557-F1-model_v2	-0.055833519	101	K	R
## 1438	AF-P35557-F1-model_v2	-0.085415184	101	K	H
## 1439	AF-P35557-F1-model_v2	-0.555718064	101	K	I
## 1440	AF-P35557-F1-model_v2	-0.012453914	101	K	Q
## 1441	AF-P35557-F1-model_v2	2.025009155	101	K	P
## 1442	AF-P35557-F1-model_v2	-0.064503074	101	K	L
## 1443	AF-P35557-F1-model_v2	0.683472991	102	T	A
## 1444	AF-P35557-F1-model_v2	-0.202953219	102	T	C
## 1445	AF-P35557-F1-model_v2	1.208124161	102	T	D
## 1446	AF-P35557-F1-model_v2	0.973979354	102	T	E
## 1447	AF-P35557-F1-model_v2	0.121713758	102	T	F
## 1448	AF-P35557-F1-model_v2	0.858997643	102	T	G
## 1449	AF-P35557-F1-model_v2	0.717009723	102	T	H
## 1450	AF-P35557-F1-model_v2	-0.399411201	102	T	I
## 1451	AF-P35557-F1-model_v2	1.197899818	102	T	K
## 1452	AF-P35557-F1-model_v2	0.001336336	102	T	L
## 1453	AF-P35557-F1-model_v2	0.119283319	102	T	M
## 1454	AF-P35557-F1-model_v2	1.012690902	102	T	N
## 1455	AF-P35557-F1-model_v2	1.048298478	102	T	P
## 1456	AF-P35557-F1-model_v2	0.971182585	102	T	Q
## 1457	AF-P35557-F1-model_v2	1.179571152	102	T	R
## 1458	AF-P35557-F1-model_v2	0.401659846	102	T	S
## 1459	AF-P35557-F1-model_v2	-0.210395455	102	T	V
## 1460	AF-P35557-F1-model_v2	-0.126228571	102	T	W

## 1461	AF-P35557-F1-model_v2	0.156445801	102	T	Y
## 1462	AF-P35557-F1-model_v2	-0.613982022	103	K	I
## 1463	AF-P35557-F1-model_v2	-0.210029244	103	K	L
## 1464	AF-P35557-F1-model_v2	-0.204599261	103	K	H
## 1465	AF-P35557-F1-model_v2	-0.500536382	103	K	W
## 1466	AF-P35557-F1-model_v2	-0.193836987	103	K	M
## 1467	AF-P35557-F1-model_v2	0.129046202	103	K	A
## 1468	AF-P35557-F1-model_v2	0.181693792	103	K	N
## 1469	AF-P35557-F1-model_v2	-0.082498729	103	K	E
## 1470	AF-P35557-F1-model_v2	-0.459319174	103	K	F
## 1471	AF-P35557-F1-model_v2	0.204620779	103	K	D
## 1472	AF-P35557-F1-model_v2	0.877215862	103	K	G
## 1473	AF-P35557-F1-model_v2	-0.605621994	103	K	V
## 1474	AF-P35557-F1-model_v2	-0.524171293	103	K	C
## 1475	AF-P35557-F1-model_v2	-0.100353062	103	K	Q
## 1476	AF-P35557-F1-model_v2	-0.048602402	103	K	R
## 1477	AF-P35557-F1-model_v2	-0.559797704	103	K	Y
## 1478	AF-P35557-F1-model_v2	-0.392779171	103	K	T
## 1479	AF-P35557-F1-model_v2	1.596409559	103	K	P
## 1480	AF-P35557-F1-model_v2	-0.121356785	103	K	S
## 1481	AF-P35557-F1-model_v2	-0.256618679	104	H	I
## 1482	AF-P35557-F1-model_v2	0.074082553	104	H	M
## 1483	AF-P35557-F1-model_v2	1.363362193	104	H	P
## 1484	AF-P35557-F1-model_v2	0.719396830	104	H	K
## 1485	AF-P35557-F1-model_v2	1.001102805	104	H	D
## 1486	AF-P35557-F1-model_v2	0.194848955	104	H	E
## 1487	AF-P35557-F1-model_v2	-0.239678919	104	H	C
## 1488	AF-P35557-F1-model_v2	0.432092726	104	H	Q
## 1489	AF-P35557-F1-model_v2	1.002597570	104	H	N
## 1490	AF-P35557-F1-model_v2	1.272770643	104	H	G
## 1491	AF-P35557-F1-model_v2	0.395933717	104	H	A
## 1492	AF-P35557-F1-model_v2	0.588930726	104	H	R
## 1493	AF-P35557-F1-model_v2	0.191367567	104	H	L
## 1494	AF-P35557-F1-model_v2	0.399242610	104	H	S
## 1495	AF-P35557-F1-model_v2	-0.487973034	104	H	F
## 1496	AF-P35557-F1-model_v2	-0.664586365	104	H	W
## 1497	AF-P35557-F1-model_v2	-0.157814562	104	H	V
## 1498	AF-P35557-F1-model_v2	-0.924908698	104	H	Y
## 1499	AF-P35557-F1-model_v2	0.385653108	104	H	T
## 1500	AF-P35557-F1-model_v2	0.006892860	105	Q	Y
## 1501	AF-P35557-F1-model_v2	0.667269647	105	Q	R
## 1502	AF-P35557-F1-model_v2	-0.116965234	105	Q	V
## 1503	AF-P35557-F1-model_v2	-0.317190707	105	Q	W
## 1504	AF-P35557-F1-model_v2	0.349735141	105	Q	S
## 1505	AF-P35557-F1-model_v2	0.208603382	105	Q	T
## 1506	AF-P35557-F1-model_v2	-0.104756415	105	Q	E
## 1507	AF-P35557-F1-model_v2	0.046655595	105	Q	F
## 1508	AF-P35557-F1-model_v2	0.282330930	105	Q	A
## 1509	AF-P35557-F1-model_v2	-0.081589520	105	Q	C
## 1510	AF-P35557-F1-model_v2	-0.170737088	105	Q	M
## 1511	AF-P35557-F1-model_v2	0.930071175	105	Q	N
## 1512	AF-P35557-F1-model_v2	2.110003948	105	Q	P
## 1513	AF-P35557-F1-model_v2	1.373305082	105	Q	G
## 1514	AF-P35557-F1-model_v2	0.784528136	105	Q	K

## 1515	AF-P35557-F1-model_v2	0.088145614	105	Q	L
## 1516	AF-P35557-F1-model_v2	-0.193822682	105	Q	I
## 1517	AF-P35557-F1-model_v2	0.412487566	105	Q	H
## 1518	AF-P35557-F1-model_v2	-0.092056036	106	M	V
## 1519	AF-P35557-F1-model_v2	0.281517863	106	M	T
## 1520	AF-P35557-F1-model_v2	-0.073001266	106	M	W
## 1521	AF-P35557-F1-model_v2	-0.061558485	106	M	Y
## 1522	AF-P35557-F1-model_v2	0.525405288	106	M	E
## 1523	AF-P35557-F1-model_v2	0.656428576	106	M	A
## 1524	AF-P35557-F1-model_v2	-0.114885449	106	M	C
## 1525	AF-P35557-F1-model_v2	0.501090646	106	M	D
## 1526	AF-P35557-F1-model_v2	0.587821126	106	M	R
## 1527	AF-P35557-F1-model_v2	0.551066399	106	M	S
## 1528	AF-P35557-F1-model_v2	1.425905347	106	M	P
## 1529	AF-P35557-F1-model_v2	0.492105603	106	M	N
## 1530	AF-P35557-F1-model_v2	0.544946551	106	M	Q
## 1531	AF-P35557-F1-model_v2	1.132829666	106	M	G
## 1532	AF-P35557-F1-model_v2	0.286970675	106	M	H
## 1533	AF-P35557-F1-model_v2	-0.296845675	106	M	I
## 1534	AF-P35557-F1-model_v2	-0.226287842	106	M	F
## 1535	AF-P35557-F1-model_v2	-0.049383879	106	M	L
## 1536	AF-P35557-F1-model_v2	0.678564787	106	M	K
## 1537	AF-P35557-F1-model_v2	2.361351013	107	Y	A
## 1538	AF-P35557-F1-model_v2	1.404459476	107	Y	C
## 1539	AF-P35557-F1-model_v2	2.310126305	107	Y	D
## 1540	AF-P35557-F1-model_v2	2.284131527	107	Y	E
## 1541	AF-P35557-F1-model_v2	0.650220037	107	Y	F
## 1542	AF-P35557-F1-model_v2	2.428860426	107	Y	G
## 1543	AF-P35557-F1-model_v2	1.221830487	107	Y	H
## 1544	AF-P35557-F1-model_v2	1.817607403	107	Y	I
## 1545	AF-P35557-F1-model_v2	2.189108133	107	Y	K
## 1546	AF-P35557-F1-model_v2	1.896235704	107	Y	L
## 1547	AF-P35557-F1-model_v2	1.934174657	107	Y	M
## 1548	AF-P35557-F1-model_v2	2.145803928	107	Y	N
## 1549	AF-P35557-F1-model_v2	2.272178411	107	Y	P
## 1550	AF-P35557-F1-model_v2	2.237903118	107	Y	Q
## 1551	AF-P35557-F1-model_v2	2.050279140	107	Y	R
## 1552	AF-P35557-F1-model_v2	2.326753378	107	Y	S
## 1553	AF-P35557-F1-model_v2	2.232371092	107	Y	T
## 1554	AF-P35557-F1-model_v2	2.174531698	107	Y	V
## 1555	AF-P35557-F1-model_v2	0.695390224	107	Y	W
## 1556	AF-P35557-F1-model_v2	0.073579550	108	S	A
## 1557	AF-P35557-F1-model_v2	-0.216922045	108	S	C
## 1558	AF-P35557-F1-model_v2	0.079671919	108	S	D
## 1559	AF-P35557-F1-model_v2	-0.066941202	108	S	E
## 1560	AF-P35557-F1-model_v2	-0.022348702	108	S	F
## 1561	AF-P35557-F1-model_v2	0.519384503	108	S	G
## 1562	AF-P35557-F1-model_v2	-0.048197865	108	S	H
## 1563	AF-P35557-F1-model_v2	-0.224412322	108	S	I
## 1564	AF-P35557-F1-model_v2	-0.099800527	108	S	K
## 1565	AF-P35557-F1-model_v2	-0.112665951	108	S	L
## 1566	AF-P35557-F1-model_v2	0.024303794	108	S	M
## 1567	AF-P35557-F1-model_v2	0.029328406	108	S	N
## 1568	AF-P35557-F1-model_v2	0.826143980	108	S	P

## 1569	AF-P35557-F1-model_v2	-0.044344187	108	S	Q
## 1570	AF-P35557-F1-model_v2	-0.102496386	108	S	R
## 1571	AF-P35557-F1-model_v2	-0.139908493	108	S	T
## 1572	AF-P35557-F1-model_v2	-0.218641162	108	S	V
## 1573	AF-P35557-F1-model_v2	0.015258729	108	S	W
## 1574	AF-P35557-F1-model_v2	-0.015911698	108	S	Y
## 1575	AF-P35557-F1-model_v2	2.767639637	109	I	E
## 1576	AF-P35557-F1-model_v2	2.723901987	109	I	Q
## 1577	AF-P35557-F1-model_v2	2.806938410	109	I	D
## 1578	AF-P35557-F1-model_v2	2.646668196	109	I	N
## 1579	AF-P35557-F1-model_v2	2.650813341	109	I	P
## 1580	AF-P35557-F1-model_v2	1.530417442	109	I	C
## 1581	AF-P35557-F1-model_v2	1.255064368	109	I	M
## 1582	AF-P35557-F1-model_v2	2.661360741	109	I	S
## 1583	AF-P35557-F1-model_v2	0.744131804	109	I	L
## 1584	AF-P35557-F1-model_v2	1.960928917	109	I	W
## 1585	AF-P35557-F1-model_v2	2.651988745	109	I	R
## 1586	AF-P35557-F1-model_v2	1.919474006	109	I	Y
## 1587	AF-P35557-F1-model_v2	0.656344652	109	I	V
## 1588	AF-P35557-F1-model_v2	1.302719116	109	I	F
## 1589	AF-P35557-F1-model_v2	2.190986872	109	I	A
## 1590	AF-P35557-F1-model_v2	2.714838028	109	I	K
## 1591	AF-P35557-F1-model_v2	2.567629814	109	I	H
## 1592	AF-P35557-F1-model_v2	2.764329195	109	I	G
## 1593	AF-P35557-F1-model_v2	2.161541462	109	I	T
## 1594	AF-P35557-F1-model_v2	1.772745967	110	P	Y
## 1595	AF-P35557-F1-model_v2	1.725625753	110	P	S
## 1596	AF-P35557-F1-model_v2	2.055557728	110	P	T
## 1597	AF-P35557-F1-model_v2	1.829833627	110	P	W
## 1598	AF-P35557-F1-model_v2	1.923594594	110	P	R
## 1599	AF-P35557-F1-model_v2	1.248934388	110	P	C
## 1600	AF-P35557-F1-model_v2	1.911267042	110	P	D
## 1601	AF-P35557-F1-model_v2	2.079575777	110	P	V
## 1602	AF-P35557-F1-model_v2	1.958138943	110	P	A
## 1603	AF-P35557-F1-model_v2	1.828192234	110	P	H
## 1604	AF-P35557-F1-model_v2	1.713242769	110	P	L
## 1605	AF-P35557-F1-model_v2	1.892928600	110	P	M
## 1606	AF-P35557-F1-model_v2	1.836043477	110	P	N
## 1607	AF-P35557-F1-model_v2	2.123401403	110	P	Q
## 1608	AF-P35557-F1-model_v2	2.228024960	110	P	G
## 1609	AF-P35557-F1-model_v2	1.930501461	110	P	I
## 1610	AF-P35557-F1-model_v2	2.217086077	110	P	E
## 1611	AF-P35557-F1-model_v2	1.968245864	110	P	F
## 1612	AF-P35557-F1-model_v2	1.884971619	110	P	K
## 1613	AF-P35557-F1-model_v2	-0.423738480	111	E	Y
## 1614	AF-P35557-F1-model_v2	-0.068202794	111	E	T
## 1615	AF-P35557-F1-model_v2	0.467036873	111	E	G
## 1616	AF-P35557-F1-model_v2	-0.448047996	111	E	W
## 1617	AF-P35557-F1-model_v2	-0.481812239	111	E	C
## 1618	AF-P35557-F1-model_v2	-0.482860446	111	E	F
## 1619	AF-P35557-F1-model_v2	-0.099408090	111	E	A
## 1620	AF-P35557-F1-model_v2	0.236039296	111	E	D
## 1621	AF-P35557-F1-model_v2	-0.410208106	111	E	V
## 1622	AF-P35557-F1-model_v2	-0.355338752	111	E	R

## 1623	AF-P35557-F1-model_v2	-0.292704046	111	E	H
## 1624	AF-P35557-F1-model_v2	-0.593480110	111	E	I
## 1625	AF-P35557-F1-model_v2	-0.380949974	111	E	M
## 1626	AF-P35557-F1-model_v2	0.008919567	111	E	S
## 1627	AF-P35557-F1-model_v2	-0.130267203	111	E	Q
## 1628	AF-P35557-F1-model_v2	-0.049806952	111	E	N
## 1629	AF-P35557-F1-model_v2	-0.334416151	111	E	K
## 1630	AF-P35557-F1-model_v2	0.063709378	111	E	P
## 1631	AF-P35557-F1-model_v2	-0.565823674	111	E	L
## 1632	AF-P35557-F1-model_v2	-0.040378273	112	D	S
## 1633	AF-P35557-F1-model_v2	0.074869633	112	D	M
## 1634	AF-P35557-F1-model_v2	0.222448289	112	D	G
## 1635	AF-P35557-F1-model_v2	-0.200469792	112	D	W
## 1636	AF-P35557-F1-model_v2	0.224975288	112	D	N
## 1637	AF-P35557-F1-model_v2	0.112373650	112	D	L
## 1638	AF-P35557-F1-model_v2	0.907046020	112	D	P
## 1639	AF-P35557-F1-model_v2	-0.039112270	112	D	F
## 1640	AF-P35557-F1-model_v2	0.134430885	112	D	T
## 1641	AF-P35557-F1-model_v2	0.004321933	112	D	V
## 1642	AF-P35557-F1-model_v2	0.028642952	112	D	K
## 1643	AF-P35557-F1-model_v2	0.014954805	112	D	I
## 1644	AF-P35557-F1-model_v2	-0.236506641	112	D	Y
## 1645	AF-P35557-F1-model_v2	-0.311660945	112	D	E
## 1646	AF-P35557-F1-model_v2	-0.298607886	112	D	A
## 1647	AF-P35557-F1-model_v2	-0.108262360	112	D	Q
## 1648	AF-P35557-F1-model_v2	-0.042615294	112	D	R
## 1649	AF-P35557-F1-model_v2	-0.107643604	112	D	H
## 1650	AF-P35557-F1-model_v2	-0.259928107	112	D	C
## 1651	AF-P35557-F1-model_v2	1.052491546	113	A	K
## 1652	AF-P35557-F1-model_v2	0.352618098	113	A	C
## 1653	AF-P35557-F1-model_v2	2.232127905	113	A	E
## 1654	AF-P35557-F1-model_v2	1.081852078	113	A	T
## 1655	AF-P35557-F1-model_v2	0.156735182	113	A	V
## 1656	AF-P35557-F1-model_v2	1.015909910	113	A	R
## 1657	AF-P35557-F1-model_v2	1.052347422	113	A	S
## 1658	AF-P35557-F1-model_v2	0.492463350	113	A	I
## 1659	AF-P35557-F1-model_v2	0.839516163	113	A	M
## 1660	AF-P35557-F1-model_v2	0.983629465	113	A	H
## 1661	AF-P35557-F1-model_v2	0.717658341	113	A	L
## 1662	AF-P35557-F1-model_v2	1.206662059	113	A	W
## 1663	AF-P35557-F1-model_v2	1.705565572	113	A	G
## 1664	AF-P35557-F1-model_v2	0.766053677	113	A	F
## 1665	AF-P35557-F1-model_v2	0.636861145	113	A	Y
## 1666	AF-P35557-F1-model_v2	2.455771923	113	A	P
## 1667	AF-P35557-F1-model_v2	1.494238615	113	A	N
## 1668	AF-P35557-F1-model_v2	1.384581447	113	A	Q
## 1669	AF-P35557-F1-model_v2	2.991897583	114	M	P
## 1670	AF-P35557-F1-model_v2	0.562918663	114	M	Q
## 1671	AF-P35557-F1-model_v2	1.142435551	114	M	S
## 1672	AF-P35557-F1-model_v2	1.183139086	114	M	N
## 1673	AF-P35557-F1-model_v2	0.965945959	114	M	A
## 1674	AF-P35557-F1-model_v2	-0.626050472	114	M	R
## 1675	AF-P35557-F1-model_v2	0.052972078	114	M	L
## 1676	AF-P35557-F1-model_v2	1.077239037	114	M	Y

## 1677	AF-P35557-F1-model_v2	0.869823098	114	M	F
## 1678	AF-P35557-F1-model_v2	1.949763775	114	M	G
## 1679	AF-P35557-F1-model_v2	0.605218589	114	M	C
## 1680	AF-P35557-F1-model_v2	2.329094648	114	M	D
## 1681	AF-P35557-F1-model_v2	1.055893898	114	M	W
## 1682	AF-P35557-F1-model_v2	1.799896002	114	M	E
## 1683	AF-P35557-F1-model_v2	1.072832465	114	M	H
## 1684	AF-P35557-F1-model_v2	0.224236131	114	M	I
## 1685	AF-P35557-F1-model_v2	0.481608629	114	M	V
## 1686	AF-P35557-F1-model_v2	0.876441598	114	M	T
## 1687	AF-P35557-F1-model_v2	0.726440847	115	T	A
## 1688	AF-P35557-F1-model_v2	0.371567726	115	T	C
## 1689	AF-P35557-F1-model_v2	1.414015651	115	T	D
## 1690	AF-P35557-F1-model_v2	1.016249061	115	T	E
## 1691	AF-P35557-F1-model_v2	1.125488877	115	T	G
## 1692	AF-P35557-F1-model_v2	0.621694922	115	T	H
## 1693	AF-P35557-F1-model_v2	0.509970844	115	T	I
## 1694	AF-P35557-F1-model_v2	0.513764203	115	T	K
## 1695	AF-P35557-F1-model_v2	0.375115991	115	T	L
## 1696	AF-P35557-F1-model_v2	0.466562092	115	T	M
## 1697	AF-P35557-F1-model_v2	0.715035617	115	T	N
## 1698	AF-P35557-F1-model_v2	1.637775302	115	T	P
## 1699	AF-P35557-F1-model_v2	0.666885376	115	T	Q
## 1700	AF-P35557-F1-model_v2	0.460601091	115	T	R
## 1701	AF-P35557-F1-model_v2	0.535482943	115	T	S
## 1702	AF-P35557-F1-model_v2	0.586301208	115	T	V
## 1703	AF-P35557-F1-model_v2	0.699954212	115	T	W
## 1704	AF-P35557-F1-model_v2	0.588722467	115	T	Y
## 1705	AF-P35557-F1-model_v2	0.575095415	116	G	Y
## 1706	AF-P35557-F1-model_v2	0.575791419	116	G	I
## 1707	AF-P35557-F1-model_v2	0.159517407	116	G	T
## 1708	AF-P35557-F1-model_v2	0.391060710	116	G	L
## 1709	AF-P35557-F1-model_v2	0.448469520	116	G	F
## 1710	AF-P35557-F1-model_v2	1.104638696	116	G	E
## 1711	AF-P35557-F1-model_v2	0.712916493	116	G	K
## 1712	AF-P35557-F1-model_v2	0.378915370	116	G	S
## 1713	AF-P35557-F1-model_v2	0.188085437	116	G	C
## 1714	AF-P35557-F1-model_v2	0.616089225	116	G	H
## 1715	AF-P35557-F1-model_v2	0.557350755	116	G	V
## 1716	AF-P35557-F1-model_v2	1.137133360	116	G	D
## 1717	AF-P35557-F1-model_v2	0.712865591	116	G	R
## 1718	AF-P35557-F1-model_v2	0.623666704	116	G	W
## 1719	AF-P35557-F1-model_v2	0.767346621	116	G	Q
## 1720	AF-P35557-F1-model_v2	0.631920159	116	G	A
## 1721	AF-P35557-F1-model_v2	0.649357617	116	G	N
## 1722	AF-P35557-F1-model_v2	0.616453052	116	G	M
## 1723	AF-P35557-F1-model_v2	1.585143328	116	G	P
## 1724	AF-P35557-F1-model_v2	1.706667900	117	T	A
## 1725	AF-P35557-F1-model_v2	1.118117809	117	T	C
## 1726	AF-P35557-F1-model_v2	1.014737725	117	T	D
## 1727	AF-P35557-F1-model_v2	1.782802105	117	T	E
## 1728	AF-P35557-F1-model_v2	1.671771407	117	T	F
## 1729	AF-P35557-F1-model_v2	1.605413079	117	T	G
## 1730	AF-P35557-F1-model_v2	1.309578180	117	T	H

## 1731	AF-P35557-F1-model_v2	1.826740384	117	T	I
## 1732	AF-P35557-F1-model_v2	1.658300757	117	T	L
## 1733	AF-P35557-F1-model_v2	1.823469400	117	T	M
## 1734	AF-P35557-F1-model_v2	0.604284883	117	T	N
## 1735	AF-P35557-F1-model_v2	1.909027219	117	T	P
## 1736	AF-P35557-F1-model_v2	1.746700764	117	T	Q
## 1737	AF-P35557-F1-model_v2	1.535661459	117	T	R
## 1738	AF-P35557-F1-model_v2	0.444680929	117	T	S
## 1739	AF-P35557-F1-model_v2	1.625030756	117	T	V
## 1740	AF-P35557-F1-model_v2	1.774480581	117	T	W
## 1741	AF-P35557-F1-model_v2	1.574929953	117	T	Y
## 1742	AF-P35557-F1-model_v2	0.968942940	118	A	I
## 1743	AF-P35557-F1-model_v2	1.803023577	118	A	P
## 1744	AF-P35557-F1-model_v2	2.193928480	118	A	N
## 1745	AF-P35557-F1-model_v2	1.849122882	118	A	H
## 1746	AF-P35557-F1-model_v2	2.355025768	118	A	R
## 1747	AF-P35557-F1-model_v2	1.646660328	118	A	G
## 1748	AF-P35557-F1-model_v2	2.484816551	118	A	K
## 1749	AF-P35557-F1-model_v2	0.182464600	118	A	V
## 1750	AF-P35557-F1-model_v2	1.227808237	118	A	Y
## 1751	AF-P35557-F1-model_v2	1.393815875	118	A	L
## 1752	AF-P35557-F1-model_v2	2.247778177	118	A	Q
## 1753	AF-P35557-F1-model_v2	1.246929526	118	A	T
## 1754	AF-P35557-F1-model_v2	2.425150871	118	A	D
## 1755	AF-P35557-F1-model_v2	1.449170470	118	A	M
## 1756	AF-P35557-F1-model_v2	2.113346100	118	A	E
## 1757	AF-P35557-F1-model_v2	1.158326745	118	A	S
## 1758	AF-P35557-F1-model_v2	1.206544757	118	A	F
## 1759	AF-P35557-F1-model_v2	1.154638767	118	A	W
## 1760	AF-P35557-F1-model_v2	0.396706820	118	A	C
## 1761	AF-P35557-F1-model_v2	0.435328960	119	E	H
## 1762	AF-P35557-F1-model_v2	0.078475893	119	E	A
## 1763	AF-P35557-F1-model_v2	0.247963428	119	E	W
## 1764	AF-P35557-F1-model_v2	0.377571046	119	E	V
## 1765	AF-P35557-F1-model_v2	0.453277826	119	E	N
## 1766	AF-P35557-F1-model_v2	1.298045635	119	E	P
## 1767	AF-P35557-F1-model_v2	0.193503380	119	E	L
## 1768	AF-P35557-F1-model_v2	0.399891078	119	E	Y
## 1769	AF-P35557-F1-model_v2	0.218958139	119	E	M
## 1770	AF-P35557-F1-model_v2	0.264444590	119	E	D
## 1771	AF-P35557-F1-model_v2	0.299479604	119	E	I
## 1772	AF-P35557-F1-model_v2	0.164156795	119	E	K
## 1773	AF-P35557-F1-model_v2	0.663433194	119	E	G
## 1774	AF-P35557-F1-model_v2	0.325184584	119	E	T
## 1775	AF-P35557-F1-model_v2	0.277188659	119	E	S
## 1776	AF-P35557-F1-model_v2	0.080868244	119	E	Q
## 1777	AF-P35557-F1-model_v2	0.160252690	119	E	C
## 1778	AF-P35557-F1-model_v2	0.491738021	119	E	F
## 1779	AF-P35557-F1-model_v2	0.168668747	119	E	R
## 1780	AF-P35557-F1-model_v2	0.989848673	120	M	Y
## 1781	AF-P35557-F1-model_v2	0.552160382	120	M	V
## 1782	AF-P35557-F1-model_v2	0.836802781	120	M	W
## 1783	AF-P35557-F1-model_v2	0.707875669	120	M	S
## 1784	AF-P35557-F1-model_v2	0.520524800	120	M	T

## 1785	AF-P35557-F1-model_v2	0.741300881	120	M	F
## 1786	AF-P35557-F1-model_v2	0.685588002	120	M	R
## 1787	AF-P35557-F1-model_v2	1.110183954	120	M	G
## 1788	AF-P35557-F1-model_v2	0.504774511	120	M	C
## 1789	AF-P35557-F1-model_v2	0.427050054	120	M	E
## 1790	AF-P35557-F1-model_v2	2.397064209	120	M	P
## 1791	AF-P35557-F1-model_v2	0.462185562	120	M	A
## 1792	AF-P35557-F1-model_v2	0.435820103	120	M	I
## 1793	AF-P35557-F1-model_v2	0.199504375	120	M	D
## 1794	AF-P35557-F1-model_v2	0.092199922	120	M	Q
## 1795	AF-P35557-F1-model_v2	0.765654862	120	M	H
## 1796	AF-P35557-F1-model_v2	0.712069333	120	M	K
## 1797	AF-P35557-F1-model_v2	0.165752888	120	M	L
## 1798	AF-P35557-F1-model_v2	0.660992265	120	M	N
## 1799	AF-P35557-F1-model_v2	2.581511021	121	L	R
## 1800	AF-P35557-F1-model_v2	2.487820148	121	L	S
## 1801	AF-P35557-F1-model_v2	1.262063146	121	L	C
## 1802	AF-P35557-F1-model_v2	2.281883478	121	L	T
## 1803	AF-P35557-F1-model_v2	2.540587902	121	L	G
## 1804	AF-P35557-F1-model_v2	2.546369553	121	L	D
## 1805	AF-P35557-F1-model_v2	2.486422300	121	L	Q
## 1806	AF-P35557-F1-model_v2	2.531628370	121	L	H
## 1807	AF-P35557-F1-model_v2	1.946320057	121	L	A
## 1808	AF-P35557-F1-model_v2	0.987584352	121	L	I
## 1809	AF-P35557-F1-model_v2	2.360463142	121	L	E
## 1810	AF-P35557-F1-model_v2	1.018798709	121	L	F
## 1811	AF-P35557-F1-model_v2	1.630162477	121	L	W
## 1812	AF-P35557-F1-model_v2	1.766316891	121	L	Y
## 1813	AF-P35557-F1-model_v2	1.412986755	121	L	V
## 1814	AF-P35557-F1-model_v2	2.652523041	121	L	N
## 1815	AF-P35557-F1-model_v2	2.540617228	121	L	P
## 1816	AF-P35557-F1-model_v2	2.565320969	121	L	K
## 1817	AF-P35557-F1-model_v2	2.845409632	122	F	E
## 1818	AF-P35557-F1-model_v2	2.479299307	122	F	N
## 1819	AF-P35557-F1-model_v2	2.838211298	122	F	D
## 1820	AF-P35557-F1-model_v2	2.550494671	122	F	H
## 1821	AF-P35557-F1-model_v2	2.532076836	122	F	S
## 1822	AF-P35557-F1-model_v2	2.232922316	122	F	T
## 1823	AF-P35557-F1-model_v2	2.743925810	122	F	G
## 1824	AF-P35557-F1-model_v2	1.553252220	122	F	M
## 1825	AF-P35557-F1-model_v2	2.725341797	122	F	Q
## 1826	AF-P35557-F1-model_v2	1.884945273	122	F	I
## 1827	AF-P35557-F1-model_v2	1.407353759	122	F	C
## 1828	AF-P35557-F1-model_v2	2.622635365	122	F	R
## 1829	AF-P35557-F1-model_v2	2.589111090	122	F	A
## 1830	AF-P35557-F1-model_v2	1.489495516	122	F	L
## 1831	AF-P35557-F1-model_v2	2.655765057	122	F	K
## 1832	AF-P35557-F1-model_v2	1.490545869	122	F	Y
## 1833	AF-P35557-F1-model_v2	1.584068060	122	F	W
## 1834	AF-P35557-F1-model_v2	3.025034428	122	F	P
## 1835	AF-P35557-F1-model_v2	2.018683910	122	F	V
## 1836	AF-P35557-F1-model_v2	1.216479659	123	D	Q
## 1837	AF-P35557-F1-model_v2	1.823065758	123	D	I
## 1838	AF-P35557-F1-model_v2	1.609522581	123	D	F

## 1839	AF-P35557-F1-model_v2	1.851587892	123	D	G
## 1840	AF-P35557-F1-model_v2	1.529842854	123	D	A
## 1841	AF-P35557-F1-model_v2	1.103398323	123	D	C
## 1842	AF-P35557-F1-model_v2	2.801953077	123	D	P
## 1843	AF-P35557-F1-model_v2	1.295850754	123	D	L
## 1844	AF-P35557-F1-model_v2	1.900390387	123	D	K
## 1845	AF-P35557-F1-model_v2	0.891590238	123	D	E
## 1846	AF-P35557-F1-model_v2	1.847059011	123	D	R
## 1847	AF-P35557-F1-model_v2	1.952608109	123	D	V
## 1848	AF-P35557-F1-model_v2	1.176385403	123	D	S
## 1849	AF-P35557-F1-model_v2	1.271375179	123	D	M
## 1850	AF-P35557-F1-model_v2	1.399607897	123	D	W
## 1851	AF-P35557-F1-model_v2	1.404628515	123	D	T
## 1852	AF-P35557-F1-model_v2	2.528212070	124	Y	A
## 1853	AF-P35557-F1-model_v2	1.341831565	124	Y	C
## 1854	AF-P35557-F1-model_v2	3.137354612	124	Y	D
## 1855	AF-P35557-F1-model_v2	2.893920183	124	Y	E
## 1856	AF-P35557-F1-model_v2	0.316745281	124	Y	F
## 1857	AF-P35557-F1-model_v2	2.992194891	124	Y	G
## 1858	AF-P35557-F1-model_v2	1.815830469	124	Y	H
## 1859	AF-P35557-F1-model_v2	1.888477564	124	Y	I
## 1860	AF-P35557-F1-model_v2	2.099245310	124	Y	K
## 1861	AF-P35557-F1-model_v2	1.592807055	124	Y	L
## 1862	AF-P35557-F1-model_v2	1.589817762	124	Y	M
## 1863	AF-P35557-F1-model_v2	2.593912601	124	Y	N
## 1864	AF-P35557-F1-model_v2	3.040959120	124	Y	P
## 1865	AF-P35557-F1-model_v2	2.312348843	124	Y	Q
## 1866	AF-P35557-F1-model_v2	1.859121680	124	Y	R
## 1867	AF-P35557-F1-model_v2	2.551790476	124	Y	S
## 1868	AF-P35557-F1-model_v2	2.542455912	124	Y	T
## 1869	AF-P35557-F1-model_v2	2.043690205	124	Y	V
## 1870	AF-P35557-F1-model_v2	-0.393247843	124	Y	W
## 1871	AF-P35557-F1-model_v2	2.288591862	125	I	K
## 1872	AF-P35557-F1-model_v2	2.474430084	125	I	G
## 1873	AF-P35557-F1-model_v2	0.989041090	125	I	C
## 1874	AF-P35557-F1-model_v2	1.481110334	125	I	A
## 1875	AF-P35557-F1-model_v2	2.027048826	125	I	H
## 1876	AF-P35557-F1-model_v2	0.975622773	125	I	M
## 1877	AF-P35557-F1-model_v2	2.567764997	125	I	E
## 1878	AF-P35557-F1-model_v2	2.886426449	125	I	D
## 1879	AF-P35557-F1-model_v2	0.647940159	125	I	L
## 1880	AF-P35557-F1-model_v2	0.852650881	125	I	F
## 1881	AF-P35557-F1-model_v2	0.670349956	125	I	V
## 1882	AF-P35557-F1-model_v2	1.049650311	125	I	Y
## 1883	AF-P35557-F1-model_v2	1.184440732	125	I	W
## 1884	AF-P35557-F1-model_v2	2.530538082	125	I	N
## 1885	AF-P35557-F1-model_v2	2.960959911	125	I	P
## 1886	AF-P35557-F1-model_v2	1.597247124	125	I	T
## 1887	AF-P35557-F1-model_v2	2.227235317	125	I	Q
## 1888	AF-P35557-F1-model_v2	2.097589016	125	I	S
## 1889	AF-P35557-F1-model_v2	2.303068399	125	I	R
## 1890	AF-P35557-F1-model_v2	-0.573474467	126	S	A
## 1891	AF-P35557-F1-model_v2	-0.416049778	126	S	C
## 1892	AF-P35557-F1-model_v2	1.675758481	126	S	D

## 1893	AF-P35557-F1-model_v2	1.073670864	126	S	E
## 1894	AF-P35557-F1-model_v2	-0.174375117	126	S	F
## 1895	AF-P35557-F1-model_v2	0.913135052	126	S	G
## 1896	AF-P35557-F1-model_v2	0.919028342	126	S	H
## 1897	AF-P35557-F1-model_v2	-0.848569810	126	S	I
## 1898	AF-P35557-F1-model_v2	1.085381389	126	S	K
## 1899	AF-P35557-F1-model_v2	0.015570462	126	S	L
## 1900	AF-P35557-F1-model_v2	1.470223427	126	S	N
## 1901	AF-P35557-F1-model_v2	1.321113348	126	S	P
## 1902	AF-P35557-F1-model_v2	0.913647175	126	S	R
## 1903	AF-P35557-F1-model_v2	-0.188878238	126	S	T
## 1904	AF-P35557-F1-model_v2	-0.902662456	126	S	V
## 1905	AF-P35557-F1-model_v2	0.053930461	126	S	W
## 1906	AF-P35557-F1-model_v2	-0.136157751	127	E	M
## 1907	AF-P35557-F1-model_v2	0.150929213	127	E	Y
## 1908	AF-P35557-F1-model_v2	-0.132005274	127	E	L
## 1909	AF-P35557-F1-model_v2	-0.255885363	127	E	K
## 1910	AF-P35557-F1-model_v2	0.478687555	127	E	G
## 1911	AF-P35557-F1-model_v2	0.079224885	127	E	H
## 1912	AF-P35557-F1-model_v2	0.168137848	127	E	W
## 1913	AF-P35557-F1-model_v2	0.112945437	127	E	F
## 1914	AF-P35557-F1-model_v2	-0.141872585	127	E	A
## 1915	AF-P35557-F1-model_v2	0.034394026	127	E	N
## 1916	AF-P35557-F1-model_v2	-0.008168221	127	E	I
## 1917	AF-P35557-F1-model_v2	0.119945824	127	E	V
## 1918	AF-P35557-F1-model_v2	-0.204300880	127	E	C
## 1919	AF-P35557-F1-model_v2	0.065419793	127	E	S
## 1920	AF-P35557-F1-model_v2	-0.321606517	127	E	R
## 1921	AF-P35557-F1-model_v2	2.390459061	127	E	P
## 1922	AF-P35557-F1-model_v2	0.103753984	127	E	T
## 1923	AF-P35557-F1-model_v2	-0.173364997	127	E	Q
## 1924	AF-P35557-F1-model_v2	0.709964097	128	C	T
## 1925	AF-P35557-F1-model_v2	0.422030210	128	C	A
## 1926	AF-P35557-F1-model_v2	0.282547474	128	C	V
## 1927	AF-P35557-F1-model_v2	1.475346446	128	C	K
## 1928	AF-P35557-F1-model_v2	0.275434852	128	C	L
## 1929	AF-P35557-F1-model_v2	0.170706034	128	C	I
## 1930	AF-P35557-F1-model_v2	1.002120495	128	C	S
## 1931	AF-P35557-F1-model_v2	1.640369415	128	C	N
## 1932	AF-P35557-F1-model_v2	1.597571015	128	C	P
## 1933	AF-P35557-F1-model_v2	0.215637684	128	C	M
## 1934	AF-P35557-F1-model_v2	2.145517349	128	C	D
## 1935	AF-P35557-F1-model_v2	0.584900558	128	C	W
## 1936	AF-P35557-F1-model_v2	1.430274963	128	C	Q
## 1937	AF-P35557-F1-model_v2	1.828512192	128	C	E
## 1938	AF-P35557-F1-model_v2	1.163801551	128	C	H
## 1939	AF-P35557-F1-model_v2	1.506250501	128	C	R
## 1940	AF-P35557-F1-model_v2	1.522169352	128	C	G
## 1941	AF-P35557-F1-model_v2	3.239987373	129	I	E
## 1942	AF-P35557-F1-model_v2	1.761821985	129	I	F
## 1943	AF-P35557-F1-model_v2	2.326841116	129	I	T
## 1944	AF-P35557-F1-model_v2	3.015125513	129	I	G
## 1945	AF-P35557-F1-model_v2	1.417868137	129	I	C
## 1946	AF-P35557-F1-model_v2	3.002087831	129	I	R

##	1947	AF-P35557-F1-model_v2	2.908950567	129	I	S
##	1948	AF-P35557-F1-model_v2	2.979890108	129	I	K
##	1949	AF-P35557-F1-model_v2	0.698234558	129	I	V
##	1950	AF-P35557-F1-model_v2	2.004468441	129	I	W
##	1951	AF-P35557-F1-model_v2	2.997647285	129	I	H
##	1952	AF-P35557-F1-model_v2	2.118688822	129	I	Y
##	1953	AF-P35557-F1-model_v2	0.547561169	129	I	L
##	1954	AF-P35557-F1-model_v2	3.003609419	129	I	Q
##	1955	AF-P35557-F1-model_v2	3.185714006	129	I	N
##	1956	AF-P35557-F1-model_v2	2.052037954	129	I	A
##	1957	AF-P35557-F1-model_v2	3.487926960	129	I	P
##	1958	AF-P35557-F1-model_v2	0.094851017	130	S	A
##	1959	AF-P35557-F1-model_v2	0.483123302	130	S	C
##	1960	AF-P35557-F1-model_v2	1.889165282	130	S	D
##	1961	AF-P35557-F1-model_v2	1.699752331	130	S	E
##	1962	AF-P35557-F1-model_v2	1.041793704	130	S	F
##	1963	AF-P35557-F1-model_v2	0.988985240	130	S	G
##	1964	AF-P35557-F1-model_v2	0.728905320	130	S	H
##	1965	AF-P35557-F1-model_v2	1.080054522	130	S	I
##	1966	AF-P35557-F1-model_v2	0.144299507	130	S	K
##	1967	AF-P35557-F1-model_v2	0.963500559	130	S	L
##	1968	AF-P35557-F1-model_v2	0.545504332	130	S	M
##	1969	AF-P35557-F1-model_v2	0.781988323	130	S	N
##	1970	AF-P35557-F1-model_v2	2.868839741	130	S	P
##	1971	AF-P35557-F1-model_v2	0.704342127	130	S	Q
##	1972	AF-P35557-F1-model_v2	-0.200178266	130	S	R
##	1973	AF-P35557-F1-model_v2	0.996818066	130	S	T
##	1974	AF-P35557-F1-model_v2	1.040758610	130	S	V
##	1975	AF-P35557-F1-model_v2	0.983750999	130	S	W
##	1976	AF-P35557-F1-model_v2	1.016500473	130	S	Y
##	1977	AF-P35557-F1-model_v2	0.249054313	131	D	S
##	1978	AF-P35557-F1-model_v2	0.307391822	131	D	T
##	1979	AF-P35557-F1-model_v2	0.200945795	131	D	V
##	1980	AF-P35557-F1-model_v2	0.101252496	131	D	M
##	1981	AF-P35557-F1-model_v2	0.708174825	131	D	G
##	1982	AF-P35557-F1-model_v2	0.309907198	131	D	F
##	1983	AF-P35557-F1-model_v2	0.093601525	131	D	R
##	1984	AF-P35557-F1-model_v2	2.502980232	131	D	P
##	1985	AF-P35557-F1-model_v2	0.146285176	131	D	I
##	1986	AF-P35557-F1-model_v2	-0.053034186	131	D	E
##	1987	AF-P35557-F1-model_v2	-0.029553294	131	D	C
##	1988	AF-P35557-F1-model_v2	0.273165047	131	D	W
##	1989	AF-P35557-F1-model_v2	0.058197856	131	D	L
##	1990	AF-P35557-F1-model_v2	0.329111993	131	D	Y
##	1991	AF-P35557-F1-model_v2	0.048361063	131	D	Q
##	1992	AF-P35557-F1-model_v2	0.186984777	131	D	N
##	1993	AF-P35557-F1-model_v2	0.286392868	131	D	H
##	1994	AF-P35557-F1-model_v2	0.066720366	131	D	A
##	1995	AF-P35557-F1-model_v2	0.226217687	131	D	K
##	1996	AF-P35557-F1-model_v2	2.472880840	132	F	K
##	1997	AF-P35557-F1-model_v2	2.271030664	132	F	Q
##	1998	AF-P35557-F1-model_v2	2.082849264	132	F	E
##	1999	AF-P35557-F1-model_v2	1.858943343	132	F	D
##	2000	AF-P35557-F1-model_v2	1.414505243	132	F	C

##	2001	AF-P35557-F1-model_v2	1.743870020	132	F	I
##	2002	AF-P35557-F1-model_v2	1.897925377	132	F	P
##	2003	AF-P35557-F1-model_v2	1.527498245	132	F	M
##	2004	AF-P35557-F1-model_v2	2.304020405	132	F	R
##	2005	AF-P35557-F1-model_v2	2.122883558	132	F	H
##	2006	AF-P35557-F1-model_v2	2.543473959	132	F	G
##	2007	AF-P35557-F1-model_v2	1.747856975	132	F	V
##	2008	AF-P35557-F1-model_v2	2.202004671	132	F	A
##	2009	AF-P35557-F1-model_v2	1.544256806	132	F	L
##	2010	AF-P35557-F1-model_v2	2.269397259	132	F	N
##	2011	AF-P35557-F1-model_v2	0.978930235	132	F	Y
##	2012	AF-P35557-F1-model_v2	2.064683676	132	F	T
##	2013	AF-P35557-F1-model_v2	0.772436976	132	F	W
##	2014	AF-P35557-F1-model_v2	2.092433453	132	F	S
##	2015	AF-P35557-F1-model_v2	1.248692393	133	L	I
##	2016	AF-P35557-F1-model_v2	2.886335850	133	L	N
##	2017	AF-P35557-F1-model_v2	2.668949842	133	L	G
##	2018	AF-P35557-F1-model_v2	2.707147360	133	L	H
##	2019	AF-P35557-F1-model_v2	2.768742561	133	L	S
##	2020	AF-P35557-F1-model_v2	1.494322777	133	L	C
##	2021	AF-P35557-F1-model_v2	1.965703011	133	L	Y
##	2022	AF-P35557-F1-model_v2	2.015003681	133	L	W
##	2023	AF-P35557-F1-model_v2	2.643641949	133	L	R
##	2024	AF-P35557-F1-model_v2	1.793284416	133	L	V
##	2025	AF-P35557-F1-model_v2	2.587635517	133	L	K
##	2026	AF-P35557-F1-model_v2	2.594758511	133	L	Q
##	2027	AF-P35557-F1-model_v2	2.401574612	133	L	A
##	2028	AF-P35557-F1-model_v2	2.805319309	133	L	P
##	2029	AF-P35557-F1-model_v2	2.708676100	133	L	E
##	2030	AF-P35557-F1-model_v2	2.468338490	133	L	T
##	2031	AF-P35557-F1-model_v2	2.917459488	133	L	D
##	2032	AF-P35557-F1-model_v2	0.083350420	134	D	W
##	2033	AF-P35557-F1-model_v2	-0.028645515	134	D	V
##	2034	AF-P35557-F1-model_v2	-0.110320628	134	D	I
##	2035	AF-P35557-F1-model_v2	-0.072656453	134	D	L
##	2036	AF-P35557-F1-model_v2	0.188667297	134	D	S
##	2037	AF-P35557-F1-model_v2	-0.001968980	134	D	M
##	2038	AF-P35557-F1-model_v2	0.619847178	134	D	G
##	2039	AF-P35557-F1-model_v2	0.097934246	134	D	F
##	2040	AF-P35557-F1-model_v2	0.118374646	134	D	T
##	2041	AF-P35557-F1-model_v2	0.057865858	134	D	A
##	2042	AF-P35557-F1-model_v2	0.132860065	134	D	H
##	2043	AF-P35557-F1-model_v2	-0.083510160	134	D	E
##	2044	AF-P35557-F1-model_v2	-0.003349602	134	D	Q
##	2045	AF-P35557-F1-model_v2	0.022766173	134	D	R
##	2046	AF-P35557-F1-model_v2	0.162340283	134	D	N
##	2047	AF-P35557-F1-model_v2	1.904884338	134	D	P
##	2048	AF-P35557-F1-model_v2	-0.137529075	134	D	C
##	2049	AF-P35557-F1-model_v2	0.339867175	135	K	V
##	2050	AF-P35557-F1-model_v2	0.345453322	135	K	H
##	2051	AF-P35557-F1-model_v2	0.219138443	135	K	Y
##	2052	AF-P35557-F1-model_v2	0.563201964	135	K	G
##	2053	AF-P35557-F1-model_v2	0.231601655	135	K	S
##	2054	AF-P35557-F1-model_v2	0.409695745	135	K	T

##	2055	AF-P35557-F1-model_v2	0.194418252	135	K	F
##	2056	AF-P35557-F1-model_v2	-0.031132877	135	K	C
##	2057	AF-P35557-F1-model_v2	0.174746394	135	K	W
##	2058	AF-P35557-F1-model_v2	-0.083475649	135	K	A
##	2059	AF-P35557-F1-model_v2	-0.059885681	135	K	M
##	2060	AF-P35557-F1-model_v2	-0.025279462	135	K	R
##	2061	AF-P35557-F1-model_v2	0.571479082	135	K	D
##	2062	AF-P35557-F1-model_v2	-0.184506595	135	K	L
##	2063	AF-P35557-F1-model_v2	0.254411697	135	K	E
##	2064	AF-P35557-F1-model_v2	0.120038688	135	K	I
##	2065	AF-P35557-F1-model_v2	0.153605223	135	K	Q
##	2066	AF-P35557-F1-model_v2	1.605190516	135	K	P
##	2067	AF-P35557-F1-model_v2	0.252840519	136	H	F
##	2068	AF-P35557-F1-model_v2	2.337826252	136	H	P
##	2069	AF-P35557-F1-model_v2	0.771042645	136	H	Q
##	2070	AF-P35557-F1-model_v2	1.387449145	136	H	G
##	2071	AF-P35557-F1-model_v2	0.526392519	136	H	E
##	2072	AF-P35557-F1-model_v2	1.372548461	136	H	T
##	2073	AF-P35557-F1-model_v2	0.906125665	136	H	I
##	2074	AF-P35557-F1-model_v2	1.371231198	136	H	R
##	2075	AF-P35557-F1-model_v2	1.084500551	136	H	S
##	2076	AF-P35557-F1-model_v2	0.590657592	136	H	N
##	2077	AF-P35557-F1-model_v2	0.747052312	136	H	A
##	2078	AF-P35557-F1-model_v2	1.054477453	136	H	V
##	2079	AF-P35557-F1-model_v2	1.344596267	136	H	D
##	2080	AF-P35557-F1-model_v2	0.067559123	136	H	M
##	2081	AF-P35557-F1-model_v2	-0.290379167	136	H	W
##	2082	AF-P35557-F1-model_v2	-0.025555968	136	H	C
##	2083	AF-P35557-F1-model_v2	1.474649072	136	H	K
##	2084	AF-P35557-F1-model_v2	-0.381188512	136	H	Y
##	2085	AF-P35557-F1-model_v2	0.006547928	136	H	L
##	2086	AF-P35557-F1-model_v2	0.493135393	137	Q	L
##	2087	AF-P35557-F1-model_v2	0.223046958	137	Q	M
##	2088	AF-P35557-F1-model_v2	1.656132460	137	Q	P
##	2089	AF-P35557-F1-model_v2	0.454805255	137	Q	R
##	2090	AF-P35557-F1-model_v2	0.330489576	137	Q	A
##	2091	AF-P35557-F1-model_v2	-0.097037077	137	Q	N
##	2092	AF-P35557-F1-model_v2	0.291057885	137	Q	E
##	2093	AF-P35557-F1-model_v2	0.185931981	137	Q	K
##	2094	AF-P35557-F1-model_v2	0.578064799	137	Q	W
##	2095	AF-P35557-F1-model_v2	-0.061948776	137	Q	C
##	2096	AF-P35557-F1-model_v2	1.096873283	137	Q	I
##	2097	AF-P35557-F1-model_v2	0.964656353	137	Q	T
##	2098	AF-P35557-F1-model_v2	0.499862611	137	Q	F
##	2099	AF-P35557-F1-model_v2	0.559580982	137	Q	Y
##	2100	AF-P35557-F1-model_v2	0.348844290	137	Q	S
##	2101	AF-P35557-F1-model_v2	0.113592207	137	Q	H
##	2102	AF-P35557-F1-model_v2	1.152512908	137	Q	V
##	2103	AF-P35557-F1-model_v2	-0.083180666	137	Q	G
##	2104	AF-P35557-F1-model_v2	0.778207302	138	M	C
##	2105	AF-P35557-F1-model_v2	1.233065128	138	M	A
##	2106	AF-P35557-F1-model_v2	1.796258211	138	M	R
##	2107	AF-P35557-F1-model_v2	1.629709005	138	M	S
##	2108	AF-P35557-F1-model_v2	1.121900558	138	M	V

##	2109	AF-P35557-F1-model_v2	0.659762979	138	M	W
##	2110	AF-P35557-F1-model_v2	0.434745669	138	M	I
##	2111	AF-P35557-F1-model_v2	1.762225151	138	M	D
##	2112	AF-P35557-F1-model_v2	1.576161146	138	M	T
##	2113	AF-P35557-F1-model_v2	1.283659577	138	M	Q
##	2114	AF-P35557-F1-model_v2	0.721184611	138	M	F
##	2115	AF-P35557-F1-model_v2	0.070256352	138	M	L
##	2116	AF-P35557-F1-model_v2	1.634478092	138	M	E
##	2117	AF-P35557-F1-model_v2	1.877441764	138	M	N
##	2118	AF-P35557-F1-model_v2	2.213153839	138	M	P
##	2119	AF-P35557-F1-model_v2	2.097256660	138	M	G
##	2120	AF-P35557-F1-model_v2	1.405022383	138	M	H
##	2121	AF-P35557-F1-model_v2	0.790198088	138	M	Y
##	2122	AF-P35557-F1-model_v2	0.790976048	139	K	I
##	2123	AF-P35557-F1-model_v2	0.984794497	139	K	H
##	2124	AF-P35557-F1-model_v2	1.061761618	139	K	T
##	2125	AF-P35557-F1-model_v2	1.612812996	139	K	G
##	2126	AF-P35557-F1-model_v2	1.099301696	139	K	A
##	2127	AF-P35557-F1-model_v2	0.650623083	139	K	L
##	2128	AF-P35557-F1-model_v2	1.123160124	139	K	V
##	2129	AF-P35557-F1-model_v2	1.444227338	139	K	W
##	2130	AF-P35557-F1-model_v2	0.688489556	139	K	M
##	2131	AF-P35557-F1-model_v2	1.763954043	139	K	P
##	2132	AF-P35557-F1-model_v2	1.211904049	139	K	Y
##	2133	AF-P35557-F1-model_v2	0.841975212	139	K	C
##	2134	AF-P35557-F1-model_v2	1.986308932	139	K	D
##	2135	AF-P35557-F1-model_v2	0.993027687	139	K	N
##	2136	AF-P35557-F1-model_v2	1.220103860	139	K	F
##	2137	AF-P35557-F1-model_v2	0.744526148	139	K	Q
##	2138	AF-P35557-F1-model_v2	1.845211506	139	K	E
##	2139	AF-P35557-F1-model_v2	0.995679200	139	K	S
##	2140	AF-P35557-F1-model_v2	0.074646592	139	K	R
##	2141	AF-P35557-F1-model_v2	-0.035304248	140	H	E
##	2142	AF-P35557-F1-model_v2	0.920715511	140	H	P
##	2143	AF-P35557-F1-model_v2	0.539751053	140	H	I
##	2144	AF-P35557-F1-model_v2	0.181278765	140	H	M
##	2145	AF-P35557-F1-model_v2	0.050941765	140	H	F
##	2146	AF-P35557-F1-model_v2	-0.221054077	140	H	D
##	2147	AF-P35557-F1-model_v2	0.074683011	140	H	Q
##	2148	AF-P35557-F1-model_v2	0.338867217	140	H	L
##	2149	AF-P35557-F1-model_v2	-0.248636723	140	H	C
##	2150	AF-P35557-F1-model_v2	0.345286220	140	H	R
##	2151	AF-P35557-F1-model_v2	-0.007360280	140	H	N
##	2152	AF-P35557-F1-model_v2	-0.025078058	140	H	G
##	2153	AF-P35557-F1-model_v2	-0.009651005	140	H	W
##	2154	AF-P35557-F1-model_v2	0.091819108	140	H	A
##	2155	AF-P35557-F1-model_v2	0.284370244	140	H	K
##	2156	AF-P35557-F1-model_v2	0.029706299	140	H	Y
##	2157	AF-P35557-F1-model_v2	0.595756412	140	H	V
##	2158	AF-P35557-F1-model_v2	0.006624401	140	H	S
##	2159	AF-P35557-F1-model_v2	0.161047041	140	H	T
##	2160	AF-P35557-F1-model_v2	0.129519582	141	K	T
##	2161	AF-P35557-F1-model_v2	-0.095844686	141	K	W
##	2162	AF-P35557-F1-model_v2	-0.078545868	141	K	Y

## 2163	AF-P35557-F1-model_v2	-0.158363998	141	K	V
## 2164	AF-P35557-F1-model_v2	0.466038883	141	K	N
## 2165	AF-P35557-F1-model_v2	-0.128237903	141	K	L
## 2166	AF-P35557-F1-model_v2	0.353563726	141	K	S
## 2167	AF-P35557-F1-model_v2	1.064700603	141	K	P
## 2168	AF-P35557-F1-model_v2	0.393901408	141	K	A
## 2169	AF-P35557-F1-model_v2	-0.010044575	141	K	R
## 2170	AF-P35557-F1-model_v2	-0.204705060	141	K	C
## 2171	AF-P35557-F1-model_v2	0.528145790	141	K	E
## 2172	AF-P35557-F1-model_v2	0.205093503	141	K	Q
## 2173	AF-P35557-F1-model_v2	-0.376169622	141	K	I
## 2174	AF-P35557-F1-model_v2	0.812107682	141	K	D
## 2175	AF-P35557-F1-model_v2	0.856468678	141	K	G
## 2176	AF-P35557-F1-model_v2	0.158169568	141	K	H
## 2177	AF-P35557-F1-model_v2	-0.105780303	141	K	F
## 2178	AF-P35557-F1-model_v2	1.456966281	142	K	P
## 2179	AF-P35557-F1-model_v2	0.390222847	142	K	N
## 2180	AF-P35557-F1-model_v2	0.122259855	142	K	F
## 2181	AF-P35557-F1-model_v2	0.768580854	142	K	A
## 2182	AF-P35557-F1-model_v2	0.489347637	142	K	Q
## 2183	AF-P35557-F1-model_v2	0.085539222	142	K	Y
## 2184	AF-P35557-F1-model_v2	1.335882425	142	K	D
## 2185	AF-P35557-F1-model_v2	1.261957407	142	K	G
## 2186	AF-P35557-F1-model_v2	0.284782410	142	K	W
## 2187	AF-P35557-F1-model_v2	-0.056366563	142	K	C
## 2188	AF-P35557-F1-model_v2	0.224364042	142	K	H
## 2189	AF-P35557-F1-model_v2	1.110682011	142	K	E
## 2190	AF-P35557-F1-model_v2	0.268909872	142	K	T
## 2191	AF-P35557-F1-model_v2	0.164899707	142	K	M
## 2192	AF-P35557-F1-model_v2	-0.147764325	142	K	V
## 2193	AF-P35557-F1-model_v2	0.048786402	142	K	R
## 2194	AF-P35557-F1-model_v2	0.547622621	142	K	S
## 2195	AF-P35557-F1-model_v2	-0.045270443	142	K	L
## 2196	AF-P35557-F1-model_v2	-0.375648260	142	K	I
## 2197	AF-P35557-F1-model_v2	0.481004000	143	L	M
## 2198	AF-P35557-F1-model_v2	1.704123259	143	L	T
## 2199	AF-P35557-F1-model_v2	0.409082174	143	L	I
## 2200	AF-P35557-F1-model_v2	1.970208168	143	L	K
## 2201	AF-P35557-F1-model_v2	2.194451809	143	L	G
## 2202	AF-P35557-F1-model_v2	2.009031534	143	L	S
## 2203	AF-P35557-F1-model_v2	2.136812687	143	L	N
## 2204	AF-P35557-F1-model_v2	1.713174820	143	L	A
## 2205	AF-P35557-F1-model_v2	1.906174421	143	L	R
## 2206	AF-P35557-F1-model_v2	2.183298111	143	L	D
## 2207	AF-P35557-F1-model_v2	2.008933544	143	L	P
## 2208	AF-P35557-F1-model_v2	1.651376724	143	L	H
## 2209	AF-P35557-F1-model_v2	0.885997176	143	L	W
## 2210	AF-P35557-F1-model_v2	0.710052490	143	L	Y
## 2211	AF-P35557-F1-model_v2	1.021624446	143	L	V
## 2212	AF-P35557-F1-model_v2	1.910766363	143	L	Q
## 2213	AF-P35557-F1-model_v2	1.937016726	143	L	E
## 2214	AF-P35557-F1-model_v2	0.306095362	143	L	F
## 2215	AF-P35557-F1-model_v2	1.156105995	144	P	L
## 2216	AF-P35557-F1-model_v2	1.437248707	144	P	M

##	2217	AF-P35557-F1-model_v2	1.843267441	144	P	Q
##	2218	AF-P35557-F1-model_v2	1.510482550	144	P	R
##	2219	AF-P35557-F1-model_v2	1.579273939	144	P	A
##	2220	AF-P35557-F1-model_v2	1.598648548	144	P	N
##	2221	AF-P35557-F1-model_v2	1.400775671	144	P	H
##	2222	AF-P35557-F1-model_v2	1.720308542	144	P	I
##	2223	AF-P35557-F1-model_v2	1.421915293	144	P	W
##	2224	AF-P35557-F1-model_v2	1.399329424	144	P	Y
##	2225	AF-P35557-F1-model_v2	1.034705877	144	P	C
##	2226	AF-P35557-F1-model_v2	2.396959782	144	P	D
##	2227	AF-P35557-F1-model_v2	2.463850975	144	P	E
##	2228	AF-P35557-F1-model_v2	1.680195928	144	P	F
##	2229	AF-P35557-F1-model_v2	2.408606529	144	P	G
##	2230	AF-P35557-F1-model_v2	2.259232759	144	P	T
##	2231	AF-P35557-F1-model_v2	1.889922976	144	P	V
##	2232	AF-P35557-F1-model_v2	1.750573516	144	P	S
##	2233	AF-P35557-F1-model_v2	1.112412453	145	L	D
##	2234	AF-P35557-F1-model_v2	1.030469179	145	L	E
##	2235	AF-P35557-F1-model_v2	1.245545506	145	L	P
##	2236	AF-P35557-F1-model_v2	0.256570935	145	L	C
##	2237	AF-P35557-F1-model_v2	1.204212070	145	L	K
##	2238	AF-P35557-F1-model_v2	1.303661942	145	L	R
##	2239	AF-P35557-F1-model_v2	0.779212952	145	L	Q
##	2240	AF-P35557-F1-model_v2	1.277192235	145	L	H
##	2241	AF-P35557-F1-model_v2	1.326706409	145	L	N
##	2242	AF-P35557-F1-model_v2	0.873994291	145	L	W
##	2243	AF-P35557-F1-model_v2	1.276223660	145	L	G
##	2244	AF-P35557-F1-model_v2	0.581215382	145	L	S
##	2245	AF-P35557-F1-model_v2	0.116659522	145	L	I
##	2246	AF-P35557-F1-model_v2	-0.028438926	145	L	V
##	2247	AF-P35557-F1-model_v2	0.851866126	145	L	Y
##	2248	AF-P35557-F1-model_v2	-0.030276060	145	L	T
##	2249	AF-P35557-F1-model_v2	0.247475982	145	L	A
##	2250	AF-P35557-F1-model_v2	1.204625607	146	G	I
##	2251	AF-P35557-F1-model_v2	1.339621902	146	G	Y
##	2252	AF-P35557-F1-model_v2	2.604535341	146	G	E
##	2253	AF-P35557-F1-model_v2	0.927487612	146	G	F
##	2254	AF-P35557-F1-model_v2	2.156074286	146	G	H
##	2255	AF-P35557-F1-model_v2	2.281637430	146	G	K
##	2256	AF-P35557-F1-model_v2	1.302418828	146	G	W
##	2257	AF-P35557-F1-model_v2	1.679278374	146	G	A
##	2258	AF-P35557-F1-model_v2	2.688752413	146	G	D
##	2259	AF-P35557-F1-model_v2	1.166019678	146	G	V
##	2260	AF-P35557-F1-model_v2	1.947486520	146	G	S
##	2261	AF-P35557-F1-model_v2	1.941547394	146	G	T
##	2262	AF-P35557-F1-model_v2	2.264382839	146	G	R
##	2263	AF-P35557-F1-model_v2	2.321469784	146	G	Q
##	2264	AF-P35557-F1-model_v2	2.386823177	146	G	N
##	2265	AF-P35557-F1-model_v2	1.214937449	146	G	L
##	2266	AF-P35557-F1-model_v2	1.486166239	146	G	M
##	2267	AF-P35557-F1-model_v2	1.886596084	146	G	P
##	2268	AF-P35557-F1-model_v2	0.777919412	147	F	I
##	2269	AF-P35557-F1-model_v2	2.206325531	147	F	G
##	2270	AF-P35557-F1-model_v2	0.870875597	147	F	M

##	2271	AF-P35557-F1-model_v2	2.348519087	147	F	Q
##	2272	AF-P35557-F1-model_v2	2.429567575	147	F	E
##	2273	AF-P35557-F1-model_v2	2.229984283	147	F	H
##	2274	AF-P35557-F1-model_v2	2.349230051	147	F	K
##	2275	AF-P35557-F1-model_v2	2.285594702	147	F	R
##	2276	AF-P35557-F1-model_v2	2.285434723	147	F	P
##	2277	AF-P35557-F1-model_v2	2.673213482	147	F	D
##	2278	AF-P35557-F1-model_v2	0.894777775	147	F	W
##	2279	AF-P35557-F1-model_v2	2.439819098	147	F	N
##	2280	AF-P35557-F1-model_v2	2.217829466	147	F	S
##	2281	AF-P35557-F1-model_v2	1.054486871	147	F	C
##	2282	AF-P35557-F1-model_v2	2.044741154	147	F	T
##	2283	AF-P35557-F1-model_v2	0.638103962	147	F	L
##	2284	AF-P35557-F1-model_v2	0.948784947	147	F	V
##	2285	AF-P35557-F1-model_v2	1.919659138	147	F	A
##	2286	AF-P35557-F1-model_v2	0.194678783	148	T	A
##	2287	AF-P35557-F1-model_v2	0.297896504	148	T	C
##	2288	AF-P35557-F1-model_v2	1.180173516	148	T	D
##	2289	AF-P35557-F1-model_v2	1.055838346	148	T	E
##	2290	AF-P35557-F1-model_v2	0.731318593	148	T	F
##	2291	AF-P35557-F1-model_v2	1.022563338	148	T	G
##	2292	AF-P35557-F1-model_v2	0.997327626	148	T	H
##	2293	AF-P35557-F1-model_v2	0.566691339	148	T	I
##	2294	AF-P35557-F1-model_v2	1.116117120	148	T	K
##	2295	AF-P35557-F1-model_v2	0.750676036	148	T	L
##	2296	AF-P35557-F1-model_v2	0.697496533	148	T	M
##	2297	AF-P35557-F1-model_v2	0.995510042	148	T	N
##	2298	AF-P35557-F1-model_v2	1.300600648	148	T	P
##	2299	AF-P35557-F1-model_v2	1.094232798	148	T	Q
##	2300	AF-P35557-F1-model_v2	0.950303674	148	T	R
##	2301	AF-P35557-F1-model_v2	0.022467732	148	T	S
##	2302	AF-P35557-F1-model_v2	0.400919497	148	T	V
##	2303	AF-P35557-F1-model_v2	0.844084740	148	T	W
##	2304	AF-P35557-F1-model_v2	0.733820558	148	T	Y
##	2305	AF-P35557-F1-model_v2	2.528302431	149	F	N
##	2306	AF-P35557-F1-model_v2	2.401677608	149	F	S
##	2307	AF-P35557-F1-model_v2	2.139678955	149	F	H
##	2308	AF-P35557-F1-model_v2	2.424193382	149	F	Q
##	2309	AF-P35557-F1-model_v2	1.431109667	149	F	I
##	2310	AF-P35557-F1-model_v2	2.404351950	149	F	P
##	2311	AF-P35557-F1-model_v2	1.800059915	149	F	V
##	2312	AF-P35557-F1-model_v2	0.685633659	149	F	W
##	2313	AF-P35557-F1-model_v2	1.349765420	149	F	M
##	2314	AF-P35557-F1-model_v2	2.343899012	149	F	K
##	2315	AF-P35557-F1-model_v2	1.269333839	149	F	L
##	2316	AF-P35557-F1-model_v2	2.204468489	149	F	G
##	2317	AF-P35557-F1-model_v2	2.278027058	149	F	R
##	2318	AF-P35557-F1-model_v2	2.750105143	149	F	D
##	2319	AF-P35557-F1-model_v2	2.519401550	149	F	T
##	2320	AF-P35557-F1-model_v2	2.593134403	149	F	E
##	2321	AF-P35557-F1-model_v2	1.346930742	149	F	C
##	2322	AF-P35557-F1-model_v2	2.231609821	149	F	A
##	2323	AF-P35557-F1-model_v2	0.788174868	149	F	Y
##	2324	AF-P35557-F1-model_v2	1.301099896	179	N	A

##	2325	AF-P35557-F1-model_v2	0.385240912	179	N	C
##	2326	AF-P35557-F1-model_v2	-0.300250411	179	N	D
##	2327	AF-P35557-F1-model_v2	0.881502867	179	N	L
##	2328	AF-P35557-F1-model_v2	1.164264441	179	N	M
##	2329	AF-P35557-F1-model_v2	1.917352676	179	N	P
##	2330	AF-P35557-F1-model_v2	1.056606650	179	N	E
##	2331	AF-P35557-F1-model_v2	1.610384464	179	N	R
##	2332	AF-P35557-F1-model_v2	0.795958638	179	N	S
##	2333	AF-P35557-F1-model_v2	0.963102818	179	N	F
##	2334	AF-P35557-F1-model_v2	1.236635447	179	N	Q
##	2335	AF-P35557-F1-model_v2	0.781922400	179	N	V
##	2336	AF-P35557-F1-model_v2	0.879086852	179	N	Y
##	2337	AF-P35557-F1-model_v2	1.816480637	179	N	G
##	2338	AF-P35557-F1-model_v2	1.455217719	179	N	T
##	2339	AF-P35557-F1-model_v2	1.790479541	180	V	A
##	2340	AF-P35557-F1-model_v2	0.823095322	180	V	C
##	2341	AF-P35557-F1-model_v2	3.357157707	180	V	D
##	2342	AF-P35557-F1-model_v2	3.070019007	180	V	E
##	2343	AF-P35557-F1-model_v2	1.237310052	180	V	F
##	2344	AF-P35557-F1-model_v2	2.811874151	180	V	G
##	2345	AF-P35557-F1-model_v2	2.701434135	180	V	H
##	2346	AF-P35557-F1-model_v2	-0.119622946	180	V	I
##	2347	AF-P35557-F1-model_v2	3.109904766	180	V	K
##	2348	AF-P35557-F1-model_v2	0.362382412	180	V	L
##	2349	AF-P35557-F1-model_v2	0.827351928	180	V	M
##	2350	AF-P35557-F1-model_v2	3.016299486	180	V	N
##	2351	AF-P35557-F1-model_v2	2.960797310	180	V	P
##	2352	AF-P35557-F1-model_v2	2.903524876	180	V	Q
##	2353	AF-P35557-F1-model_v2	3.021526814	180	V	R
##	2354	AF-P35557-F1-model_v2	2.728501320	180	V	S
##	2355	AF-P35557-F1-model_v2	2.051552773	180	V	T
##	2356	AF-P35557-F1-model_v2	1.531471133	180	V	W
##	2357	AF-P35557-F1-model_v2	1.759478450	180	V	Y
##	2358	AF-P35557-F1-model_v2	1.309017658	181	V	A
##	2359	AF-P35557-F1-model_v2	0.651458144	181	V	C
##	2360	AF-P35557-F1-model_v2	2.078977108	181	V	E
##	2361	AF-P35557-F1-model_v2	1.410799623	181	V	F
##	2362	AF-P35557-F1-model_v2	2.106294394	181	V	G
##	2363	AF-P35557-F1-model_v2	2.125549316	181	V	H
##	2364	AF-P35557-F1-model_v2	0.012272716	181	V	I
##	2365	AF-P35557-F1-model_v2	1.955599904	181	V	K
##	2366	AF-P35557-F1-model_v2	0.491813064	181	V	L
##	2367	AF-P35557-F1-model_v2	0.836287379	181	V	M
##	2368	AF-P35557-F1-model_v2	2.250105143	181	V	N
##	2369	AF-P35557-F1-model_v2	2.393558502	181	V	P
##	2370	AF-P35557-F1-model_v2	2.021502495	181	V	R
##	2371	AF-P35557-F1-model_v2	1.595281243	181	V	S
##	2372	AF-P35557-F1-model_v2	0.842986584	181	V	T
##	2373	AF-P35557-F1-model_v2	1.458300352	181	V	W
##	2374	AF-P35557-F1-model_v2	1.669704199	181	V	Y
##	2375	AF-P35557-F1-model_v2	-0.084132642	182	G	Y
##	2376	AF-P35557-F1-model_v2	-0.179828137	182	G	W
##	2377	AF-P35557-F1-model_v2	-0.454541892	182	G	L
##	2378	AF-P35557-F1-model_v2	-0.408783108	182	G	V

##	2379	AF-P35557-F1-model_v2	-0.418207616	182	G	I
##	2380	AF-P35557-F1-model_v2	-0.708926320	182	G	A
##	2381	AF-P35557-F1-model_v2	-0.514507532	182	G	S
##	2382	AF-P35557-F1-model_v2	-0.459846348	182	G	N
##	2383	AF-P35557-F1-model_v2	-0.260616034	182	G	T
##	2384	AF-P35557-F1-model_v2	-0.311713308	182	G	K
##	2385	AF-P35557-F1-model_v2	1.427008271	182	G	P
##	2386	AF-P35557-F1-model_v2	-0.463312596	182	G	M
##	2387	AF-P35557-F1-model_v2	-0.840479374	182	G	D
##	2388	AF-P35557-F1-model_v2	-0.325647086	182	G	H
##	2389	AF-P35557-F1-model_v2	-0.153244257	182	G	F
##	2390	AF-P35557-F1-model_v2	-0.655154824	182	G	C
##	2391	AF-P35557-F1-model_v2	-0.627966881	182	G	Q
##	2392	AF-P35557-F1-model_v2	-0.390842766	182	G	R
##	2393	AF-P35557-F1-model_v2	-0.761046529	182	G	E
##	2394	AF-P35557-F1-model_v2	1.449720383	183	L	Y
##	2395	AF-P35557-F1-model_v2	1.676547885	183	L	V
##	2396	AF-P35557-F1-model_v2	1.357887268	183	L	W
##	2397	AF-P35557-F1-model_v2	1.889174938	183	L	A
##	2398	AF-P35557-F1-model_v2	1.203000665	183	L	C
##	2399	AF-P35557-F1-model_v2	1.110623598	183	L	F
##	2400	AF-P35557-F1-model_v2	2.446807384	183	L	N
##	2401	AF-P35557-F1-model_v2	2.537152767	183	L	D
##	2402	AF-P35557-F1-model_v2	2.308237076	183	L	T
##	2403	AF-P35557-F1-model_v2	2.076693535	183	L	R
##	2404	AF-P35557-F1-model_v2	2.106589794	183	L	Q
##	2405	AF-P35557-F1-model_v2	0.617349029	183	L	M
##	2406	AF-P35557-F1-model_v2	2.334082842	183	L	S
##	2407	AF-P35557-F1-model_v2	2.341876984	183	L	E
##	2408	AF-P35557-F1-model_v2	2.099831581	183	L	H
##	2409	AF-P35557-F1-model_v2	2.151931286	183	L	K
##	2410	AF-P35557-F1-model_v2	2.773696423	183	L	P
##	2411	AF-P35557-F1-model_v2	2.402816534	183	L	G
##	2412	AF-P35557-F1-model_v2	3.092390060	184	L	D
##	2413	AF-P35557-F1-model_v2	2.466469765	184	L	A
##	2414	AF-P35557-F1-model_v2	2.943272352	184	L	S
##	2415	AF-P35557-F1-model_v2	1.740097523	184	L	V
##	2416	AF-P35557-F1-model_v2	2.739152908	184	L	T
##	2417	AF-P35557-F1-model_v2	2.892384768	184	L	R
##	2418	AF-P35557-F1-model_v2	2.875114202	184	L	K
##	2419	AF-P35557-F1-model_v2	1.883247495	184	L	W
##	2420	AF-P35557-F1-model_v2	1.127688885	184	L	I
##	2421	AF-P35557-F1-model_v2	1.486644506	184	L	C
##	2422	AF-P35557-F1-model_v2	2.888191700	184	L	Q
##	2423	AF-P35557-F1-model_v2	2.883879662	184	L	E
##	2424	AF-P35557-F1-model_v2	2.740103245	184	L	G
##	2425	AF-P35557-F1-model_v2	1.913499594	184	L	Y
##	2426	AF-P35557-F1-model_v2	0.935021520	184	L	M
##	2427	AF-P35557-F1-model_v2	2.996634483	184	L	N
##	2428	AF-P35557-F1-model_v2	2.815792084	184	L	P
##	2429	AF-P35557-F1-model_v2	0.312943041	185	R	K
##	2430	AF-P35557-F1-model_v2	-0.132089138	185	R	L
##	2431	AF-P35557-F1-model_v2	2.522975445	185	R	P
##	2432	AF-P35557-F1-model_v2	0.465176225	185	R	Q

##	2433	AF-P35557-F1-model_v2	0.701825142	185	R	N
##	2434	AF-P35557-F1-model_v2	0.192041159	185	R	V
##	2435	AF-P35557-F1-model_v2	0.135668755	185	R	W
##	2436	AF-P35557-F1-model_v2	-0.065050960	185	R	M
##	2437	AF-P35557-F1-model_v2	0.254907906	185	R	F
##	2438	AF-P35557-F1-model_v2	1.344367027	185	R	G
##	2439	AF-P35557-F1-model_v2	0.434861243	185	R	H
##	2440	AF-P35557-F1-model_v2	-0.044560432	185	R	I
##	2441	AF-P35557-F1-model_v2	0.750081837	185	R	S
##	2442	AF-P35557-F1-model_v2	0.562719107	185	R	T
##	2443	AF-P35557-F1-model_v2	0.497639179	185	R	A
##	2444	AF-P35557-F1-model_v2	0.006970167	185	R	C
##	2445	AF-P35557-F1-model_v2	0.204587281	185	R	Y
##	2446	AF-P35557-F1-model_v2	0.645682931	185	R	E
##	2447	AF-P35557-F1-model_v2	0.908931613	185	R	D
##	2448	AF-P35557-F1-model_v2	-0.003750384	186	D	I
##	2449	AF-P35557-F1-model_v2	-0.066550195	186	D	E
##	2450	AF-P35557-F1-model_v2	0.156417072	186	D	H
##	2451	AF-P35557-F1-model_v2	2.260449409	186	D	P
##	2452	AF-P35557-F1-model_v2	0.108475208	186	D	N
##	2453	AF-P35557-F1-model_v2	-0.180487394	186	D	C
##	2454	AF-P35557-F1-model_v2	-0.180370212	186	D	A
##	2455	AF-P35557-F1-model_v2	0.568010449	186	D	G
##	2456	AF-P35557-F1-model_v2	0.229339421	186	D	T
##	2457	AF-P35557-F1-model_v2	-0.037223160	186	D	Q
##	2458	AF-P35557-F1-model_v2	-0.108063996	186	D	R
##	2459	AF-P35557-F1-model_v2	0.057704389	186	D	S
##	2460	AF-P35557-F1-model_v2	0.119640470	186	D	F
##	2461	AF-P35557-F1-model_v2	0.035457909	186	D	K
##	2462	AF-P35557-F1-model_v2	-0.086469531	186	D	M
##	2463	AF-P35557-F1-model_v2	-0.059776545	186	D	L
##	2464	AF-P35557-F1-model_v2	0.169644833	186	D	V
##	2465	AF-P35557-F1-model_v2	0.055241942	186	D	W
##	2466	AF-P35557-F1-model_v2	1.542267084	187	A	F
##	2467	AF-P35557-F1-model_v2	1.883077741	187	A	E
##	2468	AF-P35557-F1-model_v2	0.738953233	187	A	C
##	2469	AF-P35557-F1-model_v2	2.334119081	187	A	P
##	2470	AF-P35557-F1-model_v2	1.833132625	187	A	N
##	2471	AF-P35557-F1-model_v2	1.461864829	187	A	Y
##	2472	AF-P35557-F1-model_v2	1.113508940	187	A	K
##	2473	AF-P35557-F1-model_v2	1.252150774	187	A	G
##	2474	AF-P35557-F1-model_v2	1.270832300	187	A	Q
##	2475	AF-P35557-F1-model_v2	0.453533292	187	A	S
##	2476	AF-P35557-F1-model_v2	1.049509406	187	A	T
##	2477	AF-P35557-F1-model_v2	1.070298195	187	A	M
##	2478	AF-P35557-F1-model_v2	1.420395970	187	A	L
##	2479	AF-P35557-F1-model_v2	0.950390577	187	A	R
##	2480	AF-P35557-F1-model_v2	1.085768700	187	A	V
##	2481	AF-P35557-F1-model_v2	1.470253468	187	A	W
##	2482	AF-P35557-F1-model_v2	1.241114140	187	A	I
##	2483	AF-P35557-F1-model_v2	1.488210678	187	A	H
##	2484	AF-P35557-F1-model_v2	0.421635747	188	I	W
##	2485	AF-P35557-F1-model_v2	1.375921845	188	I	S
##	2486	AF-P35557-F1-model_v2	0.395697236	188	I	V

##	2487	AF-P35557-F1-model_v2	1.782600760	188	I	R
##	2488	AF-P35557-F1-model_v2	0.407775044	188	I	L
##	2489	AF-P35557-F1-model_v2	1.642262578	188	I	E
##	2490	AF-P35557-F1-model_v2	0.605986476	188	I	Y
##	2491	AF-P35557-F1-model_v2	1.757800579	188	I	D
##	2492	AF-P35557-F1-model_v2	0.572699785	188	I	M
##	2493	AF-P35557-F1-model_v2	1.207474709	188	I	A
##	2494	AF-P35557-F1-model_v2	1.931663871	188	I	P
##	2495	AF-P35557-F1-model_v2	0.360963702	188	I	F
##	2496	AF-P35557-F1-model_v2	1.678959489	188	I	K
##	2497	AF-P35557-F1-model_v2	1.172379971	188	I	T
##	2498	AF-P35557-F1-model_v2	0.499911189	188	I	C
##	2499	AF-P35557-F1-model_v2	1.338071823	188	I	H
##	2500	AF-P35557-F1-model_v2	1.573948026	188	I	G
##	2501	AF-P35557-F1-model_v2	1.507501721	188	I	Q
##	2502	AF-P35557-F1-model_v2	0.539751589	189	K	F
##	2503	AF-P35557-F1-model_v2	-0.060557723	189	K	R
##	2504	AF-P35557-F1-model_v2	0.398021221	189	K	S
##	2505	AF-P35557-F1-model_v2	0.685864806	189	K	D
##	2506	AF-P35557-F1-model_v2	0.490073502	189	K	H
##	2507	AF-P35557-F1-model_v2	0.792858303	189	K	G
##	2508	AF-P35557-F1-model_v2	0.573394120	189	K	V
##	2509	AF-P35557-F1-model_v2	0.527373254	189	K	T
##	2510	AF-P35557-F1-model_v2	0.419672608	189	K	E
##	2511	AF-P35557-F1-model_v2	0.392597079	189	K	N
##	2512	AF-P35557-F1-model_v2	0.243939281	189	K	C
##	2513	AF-P35557-F1-model_v2	0.529885888	189	K	W
##	2514	AF-P35557-F1-model_v2	0.533535659	189	K	Y
##	2515	AF-P35557-F1-model_v2	0.212324858	189	K	L
##	2516	AF-P35557-F1-model_v2	0.263304353	189	K	Q
##	2517	AF-P35557-F1-model_v2	2.120779514	189	K	P
##	2518	AF-P35557-F1-model_v2	0.168912649	189	K	A
##	2519	AF-P35557-F1-model_v2	1.352189779	190	R	H
##	2520	AF-P35557-F1-model_v2	1.419418573	190	R	I
##	2521	AF-P35557-F1-model_v2	1.708504796	190	R	F
##	2522	AF-P35557-F1-model_v2	1.456299901	190	R	C
##	2523	AF-P35557-F1-model_v2	2.318775177	190	R	D
##	2524	AF-P35557-F1-model_v2	2.096098423	190	R	E
##	2525	AF-P35557-F1-model_v2	2.078211069	190	R	G
##	2526	AF-P35557-F1-model_v2	1.496856928	190	R	T
##	2527	AF-P35557-F1-model_v2	1.641266346	190	R	V
##	2528	AF-P35557-F1-model_v2	1.822112203	190	R	W
##	2529	AF-P35557-F1-model_v2	1.386252880	190	R	S
##	2530	AF-P35557-F1-model_v2	1.347218037	190	R	A
##	2531	AF-P35557-F1-model_v2	0.573382616	190	R	K
##	2532	AF-P35557-F1-model_v2	1.380471230	190	R	L
##	2533	AF-P35557-F1-model_v2	1.666589499	190	R	Y
##	2534	AF-P35557-F1-model_v2	1.405566931	190	R	N
##	2535	AF-P35557-F1-model_v2	3.279823303	190	R	P
##	2536	AF-P35557-F1-model_v2	1.374910355	190	R	Q
##	2537	AF-P35557-F1-model_v2	1.325556993	190	R	M
##	2538	AF-P35557-F1-model_v2	1.999045491	191	R	V
##	2539	AF-P35557-F1-model_v2	1.897894740	191	R	N
##	2540	AF-P35557-F1-model_v2	1.787642002	191	R	Q

##	2541	AF-P35557-F1-model_v2	1.899733782	191	R	S
##	2542	AF-P35557-F1-model_v2	1.997827172	191	R	T
##	2543	AF-P35557-F1-model_v2	2.709229708	191	R	P
##	2544	AF-P35557-F1-model_v2	1.696620226	191	R	W
##	2545	AF-P35557-F1-model_v2	1.626123190	191	R	Y
##	2546	AF-P35557-F1-model_v2	2.689912796	191	R	E
##	2547	AF-P35557-F1-model_v2	1.893424869	191	R	A
##	2548	AF-P35557-F1-model_v2	1.657722712	191	R	I
##	2549	AF-P35557-F1-model_v2	0.656046391	191	R	K
##	2550	AF-P35557-F1-model_v2	1.423496723	191	R	L
##	2551	AF-P35557-F1-model_v2	1.479758263	191	R	M
##	2552	AF-P35557-F1-model_v2	1.660119176	191	R	F
##	2553	AF-P35557-F1-model_v2	1.722093105	191	R	C
##	2554	AF-P35557-F1-model_v2	2.668803453	191	R	D
##	2555	AF-P35557-F1-model_v2	2.462808132	191	R	G
##	2556	AF-P35557-F1-model_v2	1.630764723	191	R	H
##	2557	AF-P35557-F1-model_v2	0.900715590	192	G	V
##	2558	AF-P35557-F1-model_v2	1.311902761	192	G	P
##	2559	AF-P35557-F1-model_v2	0.535549104	192	G	S
##	2560	AF-P35557-F1-model_v2	0.807323694	192	G	T
##	2561	AF-P35557-F1-model_v2	0.429149210	192	G	A
##	2562	AF-P35557-F1-model_v2	0.642182469	192	G	W
##	2563	AF-P35557-F1-model_v2	0.536417127	192	G	N
##	2564	AF-P35557-F1-model_v2	0.578893661	192	G	M
##	2565	AF-P35557-F1-model_v2	0.611525714	192	G	R
##	2566	AF-P35557-F1-model_v2	0.518044710	192	G	K
##	2567	AF-P35557-F1-model_v2	0.700758040	192	G	E
##	2568	AF-P35557-F1-model_v2	0.680442333	192	G	L
##	2569	AF-P35557-F1-model_v2	0.912643671	192	G	I
##	2570	AF-P35557-F1-model_v2	0.499472499	192	G	Q
##	2571	AF-P35557-F1-model_v2	0.552078187	192	G	H
##	2572	AF-P35557-F1-model_v2	0.635137260	192	G	F
##	2573	AF-P35557-F1-model_v2	0.685705602	192	G	Y
##	2574	AF-P35557-F1-model_v2	1.293756604	193	D	M
##	2575	AF-P35557-F1-model_v2	1.281451702	193	D	Q
##	2576	AF-P35557-F1-model_v2	0.931553006	193	D	T
##	2577	AF-P35557-F1-model_v2	0.408836842	193	D	N
##	2578	AF-P35557-F1-model_v2	1.327535391	193	D	K
##	2579	AF-P35557-F1-model_v2	1.274664044	193	D	L
##	2580	AF-P35557-F1-model_v2	1.128431678	193	D	F
##	2581	AF-P35557-F1-model_v2	1.452611804	193	D	V
##	2582	AF-P35557-F1-model_v2	1.341306448	193	D	R
##	2583	AF-P35557-F1-model_v2	1.082276106	193	D	G
##	2584	AF-P35557-F1-model_v2	0.649515033	193	D	S
##	2585	AF-P35557-F1-model_v2	1.125432730	193	D	E
##	2586	AF-P35557-F1-model_v2	1.327471375	193	D	W
##	2587	AF-P35557-F1-model_v2	1.412349582	193	D	Y
##	2588	AF-P35557-F1-model_v2	1.351350307	193	D	I
##	2589	AF-P35557-F1-model_v2	0.616621971	193	D	C
##	2590	AF-P35557-F1-model_v2	2.039212942	193	D	P
##	2591	AF-P35557-F1-model_v2	1.131853819	193	D	H
##	2592	AF-P35557-F1-model_v2	1.301573038	193	D	A
##	2593	AF-P35557-F1-model_v2	0.946806908	194	F	V
##	2594	AF-P35557-F1-model_v2	2.329255104	194	F	N

##	2595	AF-P35557-F1-model_v2	2.191671848	194	F	K
##	2596	AF-P35557-F1-model_v2	1.757806301	194	F	P
##	2597	AF-P35557-F1-model_v2	2.020664692	194	F	S
##	2598	AF-P35557-F1-model_v2	2.096185446	194	F	Q
##	2599	AF-P35557-F1-model_v2	2.084206343	194	F	R
##	2600	AF-P35557-F1-model_v2	0.725163579	194	F	I
##	2601	AF-P35557-F1-model_v2	1.672365785	194	F	T
##	2602	AF-P35557-F1-model_v2	1.920832038	194	F	H
##	2603	AF-P35557-F1-model_v2	1.821767211	194	F	A
##	2604	AF-P35557-F1-model_v2	2.229139328	194	F	D
##	2605	AF-P35557-F1-model_v2	0.948750019	194	F	L
##	2606	AF-P35557-F1-model_v2	0.976609230	194	F	M
##	2607	AF-P35557-F1-model_v2	1.301984549	194	F	W
##	2608	AF-P35557-F1-model_v2	2.171993256	194	F	E
##	2609	AF-P35557-F1-model_v2	2.374400377	194	F	G
##	2610	AF-P35557-F1-model_v2	0.740049481	194	F	Y
##	2611	AF-P35557-F1-model_v2	1.072219491	195	E	P
##	2612	AF-P35557-F1-model_v2	0.226722658	195	E	L
##	2613	AF-P35557-F1-model_v2	0.429257095	195	E	N
##	2614	AF-P35557-F1-model_v2	0.085316718	195	E	I
##	2615	AF-P35557-F1-model_v2	0.140060663	195	E	Y
##	2616	AF-P35557-F1-model_v2	0.489804834	195	E	R
##	2617	AF-P35557-F1-model_v2	0.134311855	195	E	S
##	2618	AF-P35557-F1-model_v2	0.272419751	195	E	Q
##	2619	AF-P35557-F1-model_v2	0.674607515	195	E	G
##	2620	AF-P35557-F1-model_v2	-0.040032327	195	E	W
##	2621	AF-P35557-F1-model_v2	0.046716869	195	E	F
##	2622	AF-P35557-F1-model_v2	0.062078774	195	E	T
##	2623	AF-P35557-F1-model_v2	0.216779411	195	E	M
##	2624	AF-P35557-F1-model_v2	0.347325921	195	E	H
##	2625	AF-P35557-F1-model_v2	-0.100368202	195	E	C
##	2626	AF-P35557-F1-model_v2	0.283730209	195	E	A
##	2627	AF-P35557-F1-model_v2	0.080296099	195	E	V
##	2628	AF-P35557-F1-model_v2	-0.072029471	196	M	L
##	2629	AF-P35557-F1-model_v2	2.537411928	196	M	N
##	2630	AF-P35557-F1-model_v2	2.391622305	196	M	G
##	2631	AF-P35557-F1-model_v2	-0.175530791	196	M	I
##	2632	AF-P35557-F1-model_v2	2.524407864	196	M	E
##	2633	AF-P35557-F1-model_v2	2.747586250	196	M	D
##	2634	AF-P35557-F1-model_v2	2.278369427	196	M	H
##	2635	AF-P35557-F1-model_v2	2.313548088	196	M	Q
##	2636	AF-P35557-F1-model_v2	1.636408329	196	M	T
##	2637	AF-P35557-F1-model_v2	1.430502176	196	M	Y
##	2638	AF-P35557-F1-model_v2	2.425116539	196	M	P
##	2639	AF-P35557-F1-model_v2	1.358882189	196	M	A
##	2640	AF-P35557-F1-model_v2	2.007499695	196	M	S
##	2641	AF-P35557-F1-model_v2	1.023551941	196	M	W
##	2642	AF-P35557-F1-model_v2	2.678958416	196	M	R
##	2643	AF-P35557-F1-model_v2	0.080079556	196	M	V
##	2644	AF-P35557-F1-model_v2	0.519277513	197	D	H
##	2645	AF-P35557-F1-model_v2	0.434791684	197	D	Q
##	2646	AF-P35557-F1-model_v2	0.823309362	197	D	R
##	2647	AF-P35557-F1-model_v2	1.373565912	197	D	G
##	2648	AF-P35557-F1-model_v2	0.219412684	197	D	F

##	2649	AF-P35557-F1-model_v2	0.316041589	197	D	L
##	2650	AF-P35557-F1-model_v2	0.947470963	197	D	K
##	2651	AF-P35557-F1-model_v2	0.511188924	197	D	S
##	2652	AF-P35557-F1-model_v2	0.183214188	197	D	E
##	2653	AF-P35557-F1-model_v2	0.048493505	197	D	W
##	2654	AF-P35557-F1-model_v2	0.617266715	197	D	T
##	2655	AF-P35557-F1-model_v2	0.340540111	197	D	M
##	2656	AF-P35557-F1-model_v2	2.218468904	197	D	P
##	2657	AF-P35557-F1-model_v2	0.295095563	197	D	V
##	2658	AF-P35557-F1-model_v2	0.227656484	197	D	I
##	2659	AF-P35557-F1-model_v2	0.526889384	197	D	A
##	2660	AF-P35557-F1-model_v2	0.558053911	197	D	N
##	2661	AF-P35557-F1-model_v2	0.069658160	197	D	C
##	2662	AF-P35557-F1-model_v2	0.627026141	198	V	A
##	2663	AF-P35557-F1-model_v2	0.168928862	198	V	C
##	2664	AF-P35557-F1-model_v2	1.543591380	198	V	E
##	2665	AF-P35557-F1-model_v2	1.206149459	198	V	G
##	2666	AF-P35557-F1-model_v2	1.042728901	198	V	H
##	2667	AF-P35557-F1-model_v2	-0.150804281	198	V	I
##	2668	AF-P35557-F1-model_v2	1.406792521	198	V	K
##	2669	AF-P35557-F1-model_v2	0.369550526	198	V	L
##	2670	AF-P35557-F1-model_v2	0.486941278	198	V	M
##	2671	AF-P35557-F1-model_v2	1.350049973	198	V	N
##	2672	AF-P35557-F1-model_v2	0.759639204	198	V	P
##	2673	AF-P35557-F1-model_v2	1.395881534	198	V	Q
##	2674	AF-P35557-F1-model_v2	1.533405304	198	V	R
##	2675	AF-P35557-F1-model_v2	1.036349416	198	V	S
##	2676	AF-P35557-F1-model_v2	0.973685980	198	V	T
##	2677	AF-P35557-F1-model_v2	0.386626780	198	V	W
##	2678	AF-P35557-F1-model_v2	0.476984501	198	V	Y
##	2679	AF-P35557-F1-model_v2	1.208378077	199	V	A
##	2680	AF-P35557-F1-model_v2	0.484642625	199	V	C
##	2681	AF-P35557-F1-model_v2	2.162755013	199	V	E
##	2682	AF-P35557-F1-model_v2	1.000173569	199	V	F
##	2683	AF-P35557-F1-model_v2	1.746574521	199	V	G
##	2684	AF-P35557-F1-model_v2	1.429337978	199	V	H
##	2685	AF-P35557-F1-model_v2	0.080496311	199	V	I
##	2686	AF-P35557-F1-model_v2	1.115460515	199	V	K
##	2687	AF-P35557-F1-model_v2	0.561808944	199	V	L
##	2688	AF-P35557-F1-model_v2	0.796440125	199	V	M
##	2689	AF-P35557-F1-model_v2	1.637484074	199	V	N
##	2690	AF-P35557-F1-model_v2	2.343824148	199	V	P
##	2691	AF-P35557-F1-model_v2	1.480378270	199	V	Q
##	2692	AF-P35557-F1-model_v2	1.066662550	199	V	R
##	2693	AF-P35557-F1-model_v2	1.256455660	199	V	S
##	2694	AF-P35557-F1-model_v2	0.844977736	199	V	T
##	2695	AF-P35557-F1-model_v2	1.188901305	199	V	W
##	2696	AF-P35557-F1-model_v2	1.128098965	199	V	Y
##	2697	AF-P35557-F1-model_v2	0.018779993	200	A	T
##	2698	AF-P35557-F1-model_v2	1.490081906	200	A	Q
##	2699	AF-P35557-F1-model_v2	0.596073985	200	A	Y
##	2700	AF-P35557-F1-model_v2	1.364875197	200	A	R
##	2701	AF-P35557-F1-model_v2	0.696337759	200	A	L
##	2702	AF-P35557-F1-model_v2	1.330560446	200	A	H

##		pdb	chain	new_position	uniprot	exposure_SS	exposure_rASA
## 1	AF-P35557-F1-model_v2	A		14	P35557	H	0.74
## 2	AF-P35557-F1-model_v2	A		14	P35557	H	0.74
## 3	AF-P35557-F1-model_v2	A		14	P35557	H	0.74
## 4	AF-P35557-F1-model_v2	A		14	P35557	H	0.74
## 5	AF-P35557-F1-model_v2	A		14	P35557	H	0.74
## 6	AF-P35557-F1-model_v2	A		14	P35557	H	0.74
## 7	AF-P35557-F1-model_v2	A		14	P35557	H	0.74
## 8	AF-P35557-F1-model_v2	A		14	P35557	H	0.74
## 9	AF-P35557-F1-model_v2	A		14	P35557	H	0.74
## 10	AF-P35557-F1-model_v2	A		14	P35557	H	0.74
## 11	AF-P35557-F1-model_v2	A		14	P35557	H	0.74
## 12	AF-P35557-F1-model_v2	A		14	P35557	H	0.74
## 13	AF-P35557-F1-model_v2	A		14	P35557	H	0.74
## 14	AF-P35557-F1-model_v2	A		14	P35557	H	0.74
## 15	AF-P35557-F1-model_v2	A		14	P35557	H	0.74
## 16	AF-P35557-F1-model_v2	A		14	P35557	H	0.74
## 17	AF-P35557-F1-model_v2	A		14	P35557	H	0.74
## 18	AF-P35557-F1-model_v2	A		14	P35557	H	0.74
## 19	AF-P35557-F1-model_v2	A		14	P35557	H	0.74
## 20	AF-P35557-F1-model_v2	A		15	P35557	H	0.38
## 21	AF-P35557-F1-model_v2	A		15	P35557	H	0.38
## 22	AF-P35557-F1-model_v2	A		15	P35557	H	0.38
## 23	AF-P35557-F1-model_v2	A		15	P35557	H	0.38
## 24	AF-P35557-F1-model_v2	A		15	P35557	H	0.38
## 25	AF-P35557-F1-model_v2	A		15	P35557	H	0.38
## 26	AF-P35557-F1-model_v2	A		15	P35557	H	0.38
## 27	AF-P35557-F1-model_v2	A		15	P35557	H	0.38
## 28	AF-P35557-F1-model_v2	A		15	P35557	H	0.38
## 29	AF-P35557-F1-model_v2	A		15	P35557	H	0.38
## 30	AF-P35557-F1-model_v2	A		15	P35557	H	0.38
## 31	AF-P35557-F1-model_v2	A		15	P35557	H	0.38
## 32	AF-P35557-F1-model_v2	A		15	P35557	H	0.38
## 33	AF-P35557-F1-model_v2	A		15	P35557	H	0.38
## 34	AF-P35557-F1-model_v2	A		15	P35557	H	0.38
## 35	AF-P35557-F1-model_v2	A		15	P35557	H	0.38
## 36	AF-P35557-F1-model_v2	A		15	P35557	H	0.38
## 37	AF-P35557-F1-model_v2	A		15	P35557	H	0.38
## 38	AF-P35557-F1-model_v2	A		16	P35557	H	0.03
## 39	AF-P35557-F1-model_v2	A		16	P35557	H	0.03
## 40	AF-P35557-F1-model_v2	A		16	P35557	H	0.03
## 41	AF-P35557-F1-model_v2	A		16	P35557	H	0.03
## 42	AF-P35557-F1-model_v2	A		16	P35557	H	0.03
## 43	AF-P35557-F1-model_v2	A		16	P35557	H	0.03
## 44	AF-P35557-F1-model_v2	A		16	P35557	H	0.03
## 45	AF-P35557-F1-model_v2	A		16	P35557	H	0.03
## 46	AF-P35557-F1-model_v2	A		16	P35557	H	0.03
## 47	AF-P35557-F1-model_v2	A		16	P35557	H	0.03
## 48	AF-P35557-F1-model_v2	A		16	P35557	H	0.03
## 49	AF-P35557-F1-model_v2	A		16	P35557	H	0.03
## 50	AF-P35557-F1-model_v2	A		16	P35557	H	0.03
## 51	AF-P35557-F1-model_v2	A		16	P35557	H	0.03
## 52	AF-P35557-F1-model_v2	A		16	P35557	H	0.03
## 53	AF-P35557-F1-model_v2	A		16	P35557	H	0.03

205

206

[illegible]

[illegible]

[illegible]

[illegible]

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212

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215

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224

225

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227

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231

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238

239

240

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243

[illegible]

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246

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[illegible]

[illegible]

[illegible]

[illegible]

##	2700	AF-P35557-F1-model_v2	A	201	P35557	E	0.01
##	2701	AF-P35557-F1-model_v2	A	201	P35557	E	0.01
##	2702	AF-P35557-F1-model_v2	A	201	P35557	E	0.01
##		spot_disorder	func_esms_residue_class		func_esms_variant_class		
##	1	0		0		1	
##	2	0		0		0	
##	3	0		0		0	
##	4	0		0		0	
##	5	0		0		0	
##	6	0		0		0	
##	7	0		0		0	
##	8	0		0		1	
##	9	0		0		0	
##	10	0		0		0	
##	11	0		0		0	
##	12	0		0		0	
##	13	0		0		0	
##	14	0		0		1	
##	15	0		0		0	
##	16	0		0		2	
##	17	0		0		0	
##	18	0		0		1	
##	19	0		0		0	
##	20	0		0		0	
##	21	0		0		2	
##	22	0		0		2	
##	23	0		0		2	
##	24	0		0		0	
##	25	0		0		1	
##	26	0		0		0	
##	27	0		0		0	
##	28	0		0		1	
##	29	0		0		0	
##	30	0		0		0	
##	31	0		0		0	
##	32	0		0		2	
##	33	0		0		2	
##	34	0		0		2	
##	35	0		0		0	
##	36	0		0		1	
##	37	0		0		0	
##	38	0		0		0	
##	39	0		0		2	
##	40	0		0		0	
##	41	0		0		2	
##	42	0		0		0	
##	43	0		0		2	
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##	48	0		0		2	
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## 93	0	4	0
## 94	0	4	2
## 95	0	4	2
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## 163	0	1	1
## 164	0	1	0
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## 167	0	4	0
## 168	0	4	2
## 169	0	4	1
## 170	0	4	2
## 171	0	4	0
## 172	0	4	2
## 173	0	4	1
## 174	0	4	1
## 175	0	4	2
## 176	0	4	2
## 177	0	4	2
## 178	0	4	1
## 179	0	4	2
## 180	0	4	2
## 181	0	4	2
## 182	0	1	1
## 183	0	1	1
## 184	0	1	1
## 185	0	1	1
## 186	0	1	1
## 187	0	1	0
## 188	0	1	1
## 189	0	1	1
## 190	0	1	1
## 191	0	1	1
## 192	0	1	1
## 193	0	1	0
## 194	0	1	1
## 195	0	1	1
## 196	0	1	2
## 197	0	1	0
## 198	0	2	2
## 199	0	2	2
## 200	0	2	2
## 201	0	2	2
## 202	0	2	1
## 203	0	2	1
## 204	0	2	2
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## 243	0	1	2
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## 246	0	1	2
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## 250	0	1	0
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## 255	0	1	1
## 256	0	1	0
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## 258	0	1	1
## 259	0	1	2
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## 261	0	1	2
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## 310	0	4	0
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## 368	0	4	2
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## 397	0	1	1
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## 399	0	1	0
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## 401	0	1	1
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## 407	0	1	1
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## 410	0	1	1
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## 413	0	4	1
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## 421	0	4	2
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## 467	0	2	2
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## 472	0	2	2
## 473	0	2	2
## 474	0	2	1
## 475	0	2	2
## 476	0	2	2
## 477	0	2	1
## 478	0	2	2
## 479	0	2	1
## 480	0	2	2
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## 485	0	1	1
## 486	0	1	2
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## 488	0	1	1
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## 494	0	1	0
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## 496	0	1	1
## 497	0	1	1
## 498	0	1	1
## 499	0	1	1
## 500	0	1	1
## 501	0	1	0
## 502	0	1	1
## 503	0	1	2
## 504	0	1	1
## 505	0	1	1
## 506	0	1	1
## 507	0	1	1
## 508	0	1	1
## 509	0	1	1
## 510	0	1	1
## 511	0	1	2
## 512	0	1	0
## 513	0	1	1
## 514	0	1	1
## 515	0	1	2
## 516	0	1	2
## 517	0	1	1
## 518	0	1	1
## 519	0	1	1
## 520	0	2	2
## 521	0	2	2
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## 29			
## 30			
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## 32			
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## 35	VUS		
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VUS

VUS

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## 102
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## 207      likely_pathogenic
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## 291      likely_pathogenic
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## 342          conflict
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## 346      likely_risk_allele
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## 509	Pathogenic	R43C, R44C, R42C
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## 1	NA 0.80007279	1.294697e-01	THR	35.702192	
## 2	NA 0.68345915	5.028595e-01	THR	35.702192	
## 3	NA 0.85957961	-1.663708e-01	THR	35.702192	
## 4	NA 0.83872826	3.827838e-01	THR	35.702192	
## 5	NA 0.65712573	6.759611e-01	THR	35.702192	
## 6	NA 0.85104311	-4.545077e-01	THR	35.702192	
## 7	NA 0.75624832	1.764430e-01	THR	35.702192	
## 8	NA 0.85226599	1.066635e-01	THR	35.702192	
## 9	NA 0.88983970	1.827619e+00	THR	35.702192	
## 10	NA 0.67085853	-7.295580e-03	THR	35.702192	
## 11	NA 0.83787563	4.157761e-01	THR	35.702192	
## 12	NA 0.97771498	4.752274e-02	THR	35.702192	
## 13	NA 0.43663514	6.796475e-01	THR	35.702192	
## 14	NA 0.81703854	6.890092e-01	THR	35.702192	
## 15	NA 0.73669287	-7.661919e-02	THR	35.702192	
## 16	NA 0.76735582	5.640736e-01	THR	35.702192	
## 17	NA 0.65940319	2.115012e-01	THR	35.702192	
## 18	NA 0.59941654	1.975158e-01	THR	35.702192	
## 19	NA 0.82366888	2.340926e-01	THR	35.702192	
## 20	NA 0.89502261	7.022977e-01	LEU	35.008988	
## 21	NA 0.74305621	3.530297e-01	LEU	35.008988	
## 22	NA 0.75755264	8.660512e-02	LEU	35.008988	
## 23	NA 0.75023854	1.500497e-01	LEU	35.008988	
## 24	NA 0.78653581	-7.717479e-01	LEU	35.008988	
## 25	NA 0.63019289	1.069691e-01	LEU	35.008988	
## 26	NA 0.86990736	6.267743e-01	LEU	35.008988	
## 27	NA 0.88289475	-2.552066e-01	LEU	35.008988	
## 28	NA 0.83996114	1.046206e+00	LEU	35.008988	
## 29	NA 0.61114911	8.469659e-01	LEU	35.008988	
## 30	NA 0.85926126	5.147299e-01	LEU	35.008988	
## 31	NA 0.75722553	2.468657e-01	LEU	35.008988	
## 32	NA 0.87823779	4.233977e-01	LEU	35.008988	

## 33	NA	0.79033022	3.607629e-01	LEU	35.008988
## 34	NA	0.75338370	8.735739e-01	LEU	35.008988
## 35	NA	0.78481075	6.770509e-01	LEU	35.008988
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## 37	NA	0.57156049	1.033126e+00	LEU	35.008988
## 38	NA	0.64256444	5.073256e-01	VAL	32.011600
## 39	NA	0.48296105	2.000687e-01	VAL	32.011600
## 40	NA	0.85373848	-3.568664e-02	VAL	32.011600
## 41	NA	0.89163551	-2.293741e-01	VAL	32.011600
## 42	NA	0.62477695	2.203900e-01	VAL	32.011600
## 43	NA	0.75738898	6.867548e-01	VAL	32.011600
## 44	NA	0.80177201	3.675666e-01	VAL	32.011600
## 45	NA	0.18962532	8.684083e-01	VAL	32.011600
## 46	NA	0.88425199	1.042025e+00	VAL	32.011600
## 47	NA	0.83261530	1.730709e+00	VAL	32.011600
## 48	NA	0.35997479	3.554377e-01	VAL	32.011600
## 49	NA	0.45415346	1.360522e-01	VAL	32.011600
## 50	NA	0.51325779	-1.755214e-01	VAL	32.011600
## 51	NA	0.62313413	5.294891e-01	VAL	32.011600
## 52	NA	0.84608840	6.951826e-01	VAL	32.011600
## 53	NA	0.43102572	6.037424e-01	VAL	32.011600
## 54	NA	0.91317073	1.205482e-01	VAL	32.011600
## 55	NA	0.74360948	4.827750e-01	VAL	32.011600
## 56	NA	0.39593535	1.271835e+00	GLU	31.072326
## 57	3594721	0.85327890	-3.446957e-01	GLU	31.072326
## 58	NA	0.73007916	2.572308e-01	GLU	31.072326
## 59	NA	0.65556136	2.787199e-02	GLU	31.072326
## 60	NA	0.82924146	-4.342347e-01	GLU	31.072326
## 61	NA	0.63023581	8.547363e-01	GLU	31.072326
## 62	NA	0.77670027	-6.817234e-01	GLU	31.072326
## 63	NA	0.86688457	3.262723e-01	GLU	31.072326
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## 65	NA	0.85150037	6.785003e-01	GLU	31.072326
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## 68	NA	0.80068726	-3.980475e-01	GLU	31.072326
## 69	NA	0.61873501	7.593516e-01	GLU	31.072326
## 70	NA	0.55931558	6.480021e-01	GLU	31.072326
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## 73	NA	0.70399165	3.595447e-01	GLU	31.072326
## 74	NA	0.83666535	-3.876525e-02	GLN	31.273546
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## 79	NA	0.79454915	-8.436908e-02	GLN	31.273546
## 80	NA	0.73940310	-9.616502e-02	GLN	31.273546
## 81	1676825	0.91843591	5.665760e-01	GLN	31.273546
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## 86	3594720	0.67199264	1.705541e-01	GLN	31.273546

## 87	NA	0.86970565	6.417499e-01	GLN	31.273546
## 88	NA	0.81729663	5.637502e-01	GLN	31.273546
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## 90	NA	0.89623556	-3.835746e-01	GLN	31.273546
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## 93	NA	0.85390399	-3.753451e-01	ILE	28.545955
## 94	NA	0.61364122	6.708929e-01	ILE	28.545955
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## 96	NA	0.84946079	6.716833e-01	ILE	28.545955
## 97	2136531	0.68974748	1.245748e+00	ILE	28.545955
## 98	NA	0.54073319	1.202095e+00	ILE	28.545955
## 99	NA	0.87864807	-8.181470e-02	ILE	28.545955
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## 114	NA	0.10720708	1.145504e+00	LEU	26.346489
## 115	NA	0.19106170	2.858180e-01	LEU	26.346489
## 116	NA	0.40997993	-2.079127e-04	LEU	26.346489
## 117	NA	0.13659850	5.635129e-02	LEU	26.346489
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## 119	NA	0.13029133	-4.548797e-03	LEU	26.346489
## 120	NA	0.22591141	1.050455e-01	LEU	26.346489
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## 130	NA	0.67823826	1.847446e-01	ALA	27.172668
## 131	NA	0.72400378	-8.363659e-01	ALA	27.172668
## 132	NA	0.85536883	1.217301e-01	ALA	27.172668
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## 148	NA 0.89151702	4.342769e-02	GLU	25.087479
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## 166	NA 0.70191350	6.207471e-01	PHE	21.972886
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## 168	NA 0.22375815	7.000568e-01	PHE	21.972886
## 169	NA 0.18224037	-3.606378e-01	PHE	21.972886
## 170	NA 0.27793712	2.672160e-01	PHE	21.972886
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## 172	NA 0.28741091	-1.500808e-02	PHE	21.972886
## 173	NA 0.14360536	-2.788068e-01	PHE	21.972886
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## 181	NA 0.09311703	-9.250631e-03	PHE	21.972886
## 182	NA 0.72800950	2.572190e-01	GLN	23.534344
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## 184	NA 0.62383760	3.334472e-02	GLN	23.534344
## 185	NA 0.83855485	3.528432e-01	GLN	23.534344
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## 193	NA 0.85381855	-8.127558e-02	GLN	23.534344
## 194	NA 0.78952532	3.445249e-01	GLN	23.534344

## 195	NA	0.72568773	2.223084e-01	GLN	23.534344
## 196	NA	0.42952058	1.711011e+00	GLN	23.534344
## 197	NA	0.85233595	3.281224e-01	GLN	23.534344
## 198	NA	0.44106113	4.698050e-01	LEU	22.455181
## 199	NA	0.65857881	1.060651e-02	LEU	22.455181
## 200	NA	0.40755727	9.317387e-01	LEU	22.455181
## 201	NA	0.42367528	5.568412e-02	LEU	22.455181
## 202	NA	0.69641917	1.071027e+00	LEU	22.455181
## 203	NA	0.73589351	-6.425422e-01	LEU	22.455181
## 204	393398	0.62923960	9.449466e-01	LEU	22.455181
## 205	NA	0.13972763	6.844492e-02	LEU	22.455181
## 206	NA	0.74175836	1.038193e-01	LEU	22.455181
## 207	NA	0.28000405	-6.372723e-01	LEU	22.455181
## 208	NA	0.60853056	2.892285e-01	LEU	22.455181
## 209	NA	0.57258278	2.378400e-01	LEU	22.455181
## 210	NA	0.69933750	1.264122e-01	LEU	22.455181
## 211	NA	0.84593939	-4.371710e-01	LEU	22.455181
## 212	NA	0.74218759	-1.699669e-01	LEU	22.455181
## 213	NA	0.55793429	2.550202e-01	LEU	22.455181
## 214	NA	0.72065098	-5.462813e-02	LEU	22.455181
## 215	NA	0.51956476	4.277134e-01	LEU	22.455181
## 216	NA	0.71909190	-1.123318e-01	LEU	22.455181
## 217	NA	0.69898959	1.960555e-01	GLN	25.193124
## 218	NA	0.89039098	2.614257e-01	GLN	25.193124
## 219	NA	0.74976553	5.460014e-01	GLN	25.193124
## 220	NA	0.76163180	3.117675e-01	GLN	25.193124
## 221	NA	0.48064735	6.991474e-01	GLN	25.193124
## 222	NA	0.88644503	1.137915e+00	GLN	25.193124
## 223	NA	0.84189908	-4.093135e-01	GLN	25.193124
## 224	NA	0.67117381	1.268129e+00	GLN	25.193124
## 225	NA	0.80216169	1.278373e+00	GLN	25.193124
## 226	NA	0.85817633	-3.821658e-01	GLN	25.193124
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## 232	NA	0.82084087	1.626213e-02	GLN	25.193124
## 233	NA	0.72076588	1.135047e+00	GLN	25.193124
## 234	NA	0.77352313	-1.130016e-01	GLN	25.193124
## 235	NA	0.83499627	-8.505443e-01	GLU	24.884848
## 236	NA	0.35481360	6.910986e-01	GLU	24.884848
## 237	NA	0.54255583	6.183356e-01	GLU	24.884848
## 238	NA	0.81629035	2.320835e-02	GLU	24.884848
## 239	NA	0.38933045	-4.735445e-01	GLU	24.884848
## 240	NA	0.33474565	3.854667e-01	GLU	24.884848
## 241	NA	0.56741843	-4.918261e-01	GLU	24.884848
## 242	NA	0.73580500	-2.989189e-01	GLU	24.884848
## 243	NA	0.40994268	-4.228047e-01	GLU	24.884848
## 244	NA	0.64861606	5.301790e-01	GLU	24.884848
## 245	NA	0.65214800	7.764776e-01	GLU	24.884848
## 246	NA	0.61807597	-2.155223e-02	GLU	24.884848
## 247	NA	0.87939577	-3.381452e-01	GLU	24.884848
## 248	NA	0.31237079	1.902498e+00	GLU	24.884848

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## 250	NA	0.70286011	1.811624e-01	GLU	24.884848
## 251	NA	0.64116137	2.877893e-01	GLU	24.884848
## 252	NA	0.86559457	1.322681e-01	GLU	24.884848
## 253	NA	0.65541126	1.159641e-01	GLU	25.522191
## 254	NA	0.52533284	9.436839e-01	GLU	25.522191
## 255	NA	0.62408938	8.114897e-02	GLU	25.522191
## 256	NA	0.74466176	5.845467e-01	GLU	25.522191
## 257	NA	0.45871468	4.772027e-01	GLU	25.522191
## 258	1172675	0.78845388	-1.894366e-02	GLU	25.522191
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## 261	NA	0.73261473	-5.555654e-01	GLU	25.522191
## 262	NA	0.85834306	8.376959e-01	GLU	25.522191
## 263	NA	0.38616943	1.280603e+00	GLU	25.522191
## 264	NA	0.90716619	1.359025e+00	GLU	25.522191
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## 266	NA	0.58150858	5.522000e-02	GLU	25.522191
## 267	NA	0.65420142	2.902340e-01	GLU	25.522191
## 268	NA	0.91558116	-1.341198e-01	GLU	25.522191
## 269	NA	0.74770692	-4.418985e-04	GLU	25.522191
## 270	NA	0.65401077	1.415573e-01	GLU	25.522191
## 271	NA	0.63118220	6.741700e-02	GLU	25.522191
## 272	NA	0.80252385	3.986336e-01	ASP	22.639960
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## 274	NA	0.75657835	8.309966e-01	ASP	22.639960
## 275	NA	0.61773898	5.411381e-01	ASP	22.639960
## 276	NA	0.65189892	1.330982e+00	ASP	22.639960
## 277	NA	0.80876672	3.958246e-01	ASP	22.639960
## 278	NA	0.53317503	3.160498e-01	ASP	22.639960
## 279	NA	0.52719081	5.977647e-01	ASP	22.639960
## 280	NA	0.64937456	1.089209e-01	ASP	22.639960
## 281	NA	0.19698059	1.146555e-01	ASP	22.639960
## 282	NA	0.91752917	4.671931e-02	ASP	22.639960
## 283	NA	0.23687843	3.700386e-01	ASP	22.639960
## 284	NA	0.38733208	-1.836044e-01	ASP	22.639960
## 285	NA	0.73552734	7.347228e-01	ASP	22.639960
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## 287	NA	0.45531185	4.364530e-02	ASP	22.639960
## 288	NA	0.81946792	-1.139968e-01	LEU	20.394276
## 289	NA	0.87294722	-3.228897e-01	LEU	20.394276
## 290	NA	0.82604470	-2.688092e-01	LEU	20.394276
## 291	NA	0.17271632	5.497698e-01	LEU	20.394276
## 292	NA	0.85335957	-8.080566e-01	LEU	20.394276
## 293	NA	0.19609530	1.320247e+00	LEU	20.394276
## 294	NA	0.76795893	7.883015e-01	LEU	20.394276
## 295	NA	0.35346918	6.146500e-01	LEU	20.394276
## 296	NA	0.52752666	5.924446e-01	LEU	20.394276
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## 298	NA	0.83719905	7.974629e-01	LEU	20.394276
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## 300	NA	0.10376202	1.322810e+00	LEU	20.394276
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## 303	NA 0.65811068	6.785511e-02	LEU	20.394276
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## 305	NA 0.87719817	-3.600545e-01	LEU	20.394276
## 306	NA 0.54757235	5.197692e-01	LYS	22.137042
## 307	NA 0.69985267	5.136119e-01	LYS	22.137042
## 308	NA 0.40289886	1.003778e+00	LYS	22.137042
## 309	NA 0.70516920	2.428510e-01	LYS	22.137042
## 310	NA 0.69989833	2.311759e-01	LYS	22.137042
## 311	NA 0.74857606	3.168006e-01	LYS	22.137042
## 312	NA 0.88066472	-9.844118e-01	LYS	22.137042
## 313	NA 0.54670148	1.031671e-01	LYS	22.137042
## 314	NA 0.79213260	-3.005451e-01	LYS	22.137042
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## 324	NA 0.75251755	3.423774e-01	LYS	21.664027
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## 342	NA 0.74474994	-1.978524e-01	VAL	17.882408
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## 346	NA 0.20341342	9.746094e-01	VAL	17.882408
## 347	NA 0.64631253	-1.016798e+00	VAL	17.882408
## 348	NA 0.82487916	-2.862098e-01	VAL	17.882408
## 349	NA 0.08325323	-1.839626e-01	VAL	17.882408
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## 360	NA	0.10492676	-1.829657e-02	MET	18.001439
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## 363	NA	0.55223825	-5.074736e-01	MET	18.001439
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## 366	NA	0.65622409	-9.135189e-02	MET	18.001439
## 367	NA	0.80867820	5.102262e-03	MET	18.001439
## 368	NA	0.78743840	-4.280442e-01	MET	18.001439
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## 371	NA	0.60750421	1.115883e+00	MET	18.001439
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## 376	NA	0.88580693	-2.261245e-01	ARG	20.294841
## 377	NA	0.74170304	6.224282e-01	ARG	18.337539
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## 386	NA	0.78706977	-3.641091e-01	ARG	18.337539
## 387	NA	0.68254883	4.697568e-01	ARG	18.337539
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## 390	NA	0.71577926	4.582048e-02	ARG	18.337539
## 391	NA	0.73276815	9.315520e-01	ARG	18.337539
## 392	NA	0.75175117	-1.807339e-01	ARG	18.337539
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## 394	NA	0.77913736	-9.365588e-02	MET	15.172323
## 395	NA	0.10331720	-8.426735e-01	MET	15.172323
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## 450	NA	0.36595676	-1.610104e-01	GLU	16.092401
## 451	NA	0.34981329	-6.155567e-01	GLU	16.092401
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## 458	NA	0.14732793	-2.189354e-01	GLU	16.092401
## 459	NA	0.73980963	7.020218e-01	GLU	16.092401
## 460	NA	0.84727232	4.307217e-01	GLU	16.092401
## 461	NA	0.16236982	1.875431e-03	GLU	16.092401
## 462	NA	0.33696208	8.416221e-01	GLU	16.092401
## 463	NA	0.69679640	1.745189e-01	GLU	16.092401
## 464	NA	0.21547587	-2.918116e-01	GLU	16.092401

## 465	NA	0.37518831	-4.553467e-01	GLU	16.092401
## 466	NA	0.66863004	-7.530764e-02	GLU	16.092401
## 467	NA	0.73461652	-6.063877e-01	GLU	16.092401
## 468	NA	0.42722094	-6.908295e-01	MET	15.322972
## 469	NA	0.69853843	1.817026e-02	MET	15.322972
## 470	NA	0.24624871	1.174474e-01	MET	15.322972
## 471	NA	0.29583364	-2.962380e-01	MET	15.322972
## 472	NA	0.67966191	4.605979e-01	MET	15.322972
## 473	NA	0.86519305	3.313570e-02	MET	15.322972
## 474	NA	0.23304970	2.900918e-01	MET	15.322972
## 475	NA	0.21752645	-3.863530e-01	MET	15.322972
## 476	NA	0.31895713	-6.613538e-02	MET	15.322972
## 477	804838	0.67622828	-3.917060e-01	MET	15.322972
## 478	NA	0.18702419	-2.622788e-01	MET	15.322972
## 479	NA	0.57264467	2.554575e-01	MET	15.322972
## 480	NA	0.78764677	-7.024443e-01	MET	15.322972
## 481	NA	0.14351024	-1.804767e-01	MET	15.322972
## 482	NA	0.74660155	2.205248e-01	MET	15.322972
## 483	NA	0.14892830	-7.784277e-02	MET	15.322972
## 484	NA	0.82488405	3.511936e-02	ASP	18.773364
## 485	NA	0.75345924	5.354714e-01	ASP	18.773364
## 486	NA	0.20796900	2.092251e-02	ASP	18.773364
## 487	NA	0.70884167	3.665324e-01	ASP	18.773364
## 488	NA	0.90884323	-3.275785e-01	ASP	18.773364
## 489	NA	0.89206443	4.126071e-01	ASP	18.773364
## 490	NA	0.75463230	3.274148e-02	ASP	18.773364
## 491	NA	0.72923971	1.065125e+00	ASP	18.773364
## 492	NA	0.85595101	9.769416e-02	ASP	18.773364
## 493	NA	0.78295765	4.018847e-01	ASP	18.773364
## 494	NA	0.85488632	4.383321e-01	ASP	18.773364
## 495	NA	0.83524794	-5.994915e-02	ASP	18.773364
## 496	NA	0.63564941	4.135054e-01	ASP	18.773364
## 497	NA	0.77773393	2.897540e-01	ASP	18.773364
## 498	NA	0.80061520	3.631823e-01	ASP	18.773364
## 499	NA	0.80978229	4.403118e-01	ASP	18.773364
## 500	NA	0.73320420	1.951119e+00	ASP	18.773364
## 501	NA	0.76531738	-6.821665e-02	ASP	18.773364
## 502	NA	0.73298689	-1.426050e-01	ARG	18.524663
## 503	NA	0.25466893	-3.165412e-01	ARG	18.524663
## 504	NA	0.87699647	-4.340992e-01	ARG	18.524663
## 505	NA	0.80780480	6.267133e-02	ARG	18.524663
## 506	NA	0.79296161	-4.303041e-02	ARG	18.524663
## 507	NA	0.80681015	6.381757e-01	ARG	18.524663
## 508	NA	0.80029098	3.936215e-03	ARG	18.524663
## 509	585911	0.84732434	2.919245e-01	ARG	18.524663
## 510	NA	0.64529216	-5.305467e-01	ARG	18.524663
## 511	NA	0.69710259	-4.568985e-02	ARG	18.524663
## 512	NA	0.90627442	-6.549181e-01	ARG	18.524663
## 513	NA	0.80827993	4.693137e-01	ARG	18.524663
## 514	NA	0.60188047	-3.736543e-01	ARG	18.524663
## 515	NA	0.47662138	9.313711e-01	ARG	18.524663
## 516	NA	0.74966432	6.349718e-01	ARG	18.524663
## 517	393453	0.52803820	3.210696e-02	ARG	18.524663
## 518	NA	0.48309445	9.585922e-01	ARG	18.524663

## 519	NA	0.39097737	4.258011e-01	ARG	18.524663
## 520	NA	0.23068559	-4.255737e-01	GLY	15.287892
## 521	NA	0.44480783	-4.089508e-01	GLY	15.287892
## 522	NA	0.31704377	3.740163e-02	GLY	15.287892
## 523	NA	0.15546737	-5.336924e-01	GLY	15.287892
## 524	NA	0.18574822	2.572450e-01	GLY	15.287892
## 525	NA	0.21803994	-3.469248e-01	GLY	15.287892
## 526	NA	0.09102746	-2.015457e-01	GLY	15.287892
## 527	NA	0.18898679	5.779577e-01	GLY	15.287892
## 528	NA	0.23757712	-2.259808e-01	GLY	15.287892
## 529	NA	0.28689061	-6.596899e-01	GLY	15.287892
## 530	NA	0.29870978	-1.286863e-01	GLY	15.287892
## 531	NA	0.14051010	-3.085664e-01	GLY	15.287892
## 532	76898	0.52192425	-9.012972e-01	GLY	15.287892
## 533	NA	0.11833542	-7.856605e-01	GLY	15.287892
## 534	NA	0.19685744	-1.222198e-01	GLY	15.287892
## 535	NA	0.43017934	2.349367e-01	GLY	15.287892
## 536	NA	0.39117888	8.401349e-03	GLY	15.287892
## 537	NA	0.31249703	5.707623e-01	LEU	16.967707
## 538	NA	0.52199635	-6.145673e-01	LEU	16.967707
## 539	NA	0.36103592	1.875097e-01	LEU	16.967707
## 540	NA	0.47237226	-3.204292e-01	LEU	16.967707
## 541	NA	0.08466123	-1.281242e-01	LEU	16.967707
## 542	NA	0.37944792	-3.834098e-01	LEU	16.967707
## 543	NA	0.67579191	-4.240849e-01	LEU	16.967707
## 544	NA	0.55782878	-7.007014e-01	LEU	16.967707
## 545	NA	0.67231275	-6.471387e-01	LEU	16.967707
## 546	NA	0.31475758	-6.015348e-01	LEU	16.967707
## 547	NA	0.42492064	-4.600263e-01	LEU	16.967707
## 548	NA	0.15168640	-3.467151e-01	LEU	16.967707
## 549	NA	0.35662607	-5.685769e-01	LEU	16.967707
## 550	429796	0.17265200	1.072314e-01	LEU	16.967707
## 551	NA	0.29176465	-2.111053e-01	LEU	16.967707
## 552	NA	0.15147072	-3.625700e-01	LEU	16.967707
## 553	NA	0.33365381	-3.424911e-01	LEU	16.967707
## 554	NA	0.71727308	2.097040e-01	ARG	20.276786
## 555	NA	0.86621563	5.571074e-01	ARG	20.276786
## 556	NA	0.75395016	-1.910745e-01	ARG	20.276786
## 557	NA	0.73827139	5.031805e-01	ARG	20.276786
## 558	NA	0.75161750	8.106140e-01	ARG	20.276786
## 559	NA	0.17800217	-6.187459e-01	ARG	20.276786
## 560	NA	0.67633283	-4.577481e-01	ARG	20.276786
## 561	NA	0.81510299	5.878344e-01	ARG	20.276786
## 562	NA	0.71066213	7.839375e-01	ARG	20.276786
## 563	NA	0.60581490	-2.202801e-01	ARG	20.276786
## 564	NA	0.62795576	3.047793e-01	ARG	20.276786
## 565	NA	0.83507180	5.348469e-01	ARG	20.276786
## 566	424481	0.86606867	-1.113957e-01	ARG	20.276786
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## 568	NA	0.59162507	1.558409e-01	ARG	20.276786
## 569	1802664	0.73984447	-4.100005e-02	ARG	20.276786
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## 573	NA 0.59365466	-2.627118e-02	LEU	21.129416
## 574	NA 0.88587782	-1.797829e-02	LEU	21.129416
## 575	NA 0.87263230	3.156919e-01	LEU	21.129416
## 576	NA 0.54329319	4.210414e-01	LEU	21.129416
## 577	NA 0.84748902	6.467682e-01	LEU	21.129416
## 578	NA 0.76542000	-1.139673e-02	LEU	21.129416
## 579	NA 0.93531995	-8.646157e-01	LEU	21.129416
## 580	NA 0.83848031	-4.862528e-01	LEU	21.129416
## 581	NA 0.81979105	3.675242e-01	LEU	21.129416
## 582	NA 0.82513797	-2.388972e-02	LEU	21.129416
## 583	NA 0.78654736	3.751935e-01	LEU	21.129416
## 584	NA 0.87576769	-1.836254e-01	LEU	21.129416
## 585	NA 0.50709260	-1.011337e-01	LEU	21.129416
## 586	NA 0.78813396	8.209624e-01	LEU	21.129416
## 587	NA 0.84287463	3.403132e-01	LEU	21.129416
## 588	NA 0.54102303	1.006129e+00	LEU	21.129416
## 589	NA 0.78038420	4.381095e-01	LEU	21.129416
## 590	NA 0.78937151	-9.704278e-02	LEU	21.129416
## 591	NA 0.82857359	7.806487e-01	LEU	21.129416
## 592	NA 0.74018001	6.694555e-01	GLU	22.955763
## 593	NA 0.83492594	-5.121386e-01	GLU	22.955763
## 594	NA 0.80856411	-5.133990e-01	GLU	22.955763
## 595	NA 0.48127183	3.637282e-02	GLU	22.955763
## 596	NA 0.71245410	5.756501e-02	GLU	22.955763
## 597	NA 0.70809027	-1.380316e-01	GLU	22.955763
## 598	NA 0.63509015	-8.113274e-02	GLU	22.955763
## 599	NA 0.84798212	7.702602e-01	GLU	22.955763
## 600	NA 0.58281943	6.303191e-01	GLU	22.955763
## 601	NA 0.64467346	7.122219e-01	GLU	22.955763
## 602	NA 0.75243572	7.989933e-02	GLU	22.955763
## 603	NA 0.76120737	3.046952e-01	GLU	22.955763
## 604	NA 0.61202497	-1.649210e-01	THR	19.965048
## 605	NA 0.65233001	-2.547115e-01	THR	19.965048
## 606	NA 0.68809979	4.402055e-01	THR	19.965048
## 607	NA 0.57639928	-4.812913e-01	THR	19.965048
## 608	NA 0.76292632	5.482493e-02	THR	19.965048
## 609	NA 0.57577777	1.005673e+00	THR	19.965048
## 610	NA 0.77240349	-6.972579e-01	THR	19.965048
## 611	NA 0.56549528	4.768906e-02	THR	19.965048
## 612	NA 0.69888298	5.039340e-01	THR	19.965048
## 613	NA 0.75971344	2.776274e-01	THR	19.965048
## 614	NA 0.28401200	2.005225e-01	THR	19.965048
## 615	NA 0.65910465	-2.926166e-01	THR	19.965048
## 616	NA 0.60053584	-5.617582e-01	THR	19.965048
## 617	NA 0.65001637	-4.433543e-01	THR	19.965048
## 618	NA 0.42831481	7.406873e-01	THR	19.965048
## 619	NA 0.65190481	4.849832e-01	THR	19.965048
## 620	NA 0.56566132	3.118676e-02	THR	19.965048
## 621	NA 0.35310549	4.549117e-01	THR	19.965048
## 622	NA 0.59173259	-3.595889e-01	HIS	16.934698
## 623	NA 0.54574037	-4.332104e-01	HIS	16.934698
## 624	NA 0.80339221	-8.805993e-01	HIS	16.934698
## 625	NA 0.75069644	-7.295012e-01	HIS	16.934698
## 626	NA 0.77278988	-7.174371e-01	HIS	16.934698

## 627	NA 0.90121772	-7.644637e-01	HIS	16.934698
## 628	NA 0.75713917	-9.089501e-01	HIS	16.934698
## 629	NA 0.47271961	-1.407103e-01	HIS	16.934698
## 630	NA 0.81382082	-8.203311e-01	HIS	16.934698
## 631	NA 0.73935625	-3.624934e-01	HIS	16.934698
## 632	NA 0.84101358	6.359484e-01	HIS	16.934698
## 633	NA 0.47473271	-1.510880e-01	HIS	16.934698
## 634	NA 0.82687234	-6.495987e-01	HIS	16.934698
## 635	NA 0.80210358	-5.542362e-01	HIS	16.934698
## 636	NA 0.70265271	-7.109206e-01	HIS	16.934698
## 637	NA 0.32269305	-4.677906e-02	HIS	16.934698
## 638	NA 0.45056470	-4.695310e-01	HIS	16.934698
## 639	NA 0.60705831	-5.414507e-01	HIS	16.934698
## 640	NA 0.78438426	-4.390281e-01	GLU	16.863008
## 641	NA 0.77491073	-5.152314e-01	GLU	16.863008
## 642	NA 0.87078809	4.711473e-02	GLU	16.863008
## 643	NA 0.96503110	1.269308e+00	GLU	16.863008
## 644	NA 0.75104571	-2.456940e-02	GLU	16.863008
## 645	NA 0.76877684	1.152671e-01	GLU	16.863008
## 646	NA 0.57115706	1.782288e-01	GLU	16.863008
## 647	NA 0.66723485	8.256296e-01	GLU	16.863008
## 648	NA 0.83969278	-1.206440e-01	GLU	16.863008
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## 650	NA 0.83317617	2.551750e-01	GLU	16.863008
## 651	NA 0.80852566	5.417857e-01	GLU	16.863008
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## 654	NA 0.74361981	4.256090e-01	GLU	16.863008
## 655	NA 0.72774490	-2.078685e-01	GLU	16.863008
## 656	NA 0.38336642	4.185839e-01	GLU	16.863008
## 657	NA 0.92627197	2.654527e-01	GLU	16.863008
## 658	NA 0.75834118	1.558908e-01	GLU	16.889670
## 659	NA 0.91563608	3.685547e-02	GLU	16.889670
## 660	NA 0.77373121	1.268839e-01	GLU	16.889670
## 661	NA 0.80131021	7.600146e-02	GLU	16.889670
## 662	NA 0.85250452	-2.970916e-01	GLU	16.889670
## 663	NA 0.86354214	-2.407052e-02	GLU	16.889670
## 664	NA 0.76773059	-6.255821e-02	GLU	16.889670
## 665	NA 0.77476836	1.466746e+00	GLU	16.889670
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## 667	NA 0.82207474	9.156012e-02	GLU	16.889670
## 668	NA 0.32616533	6.508162e-01	GLU	16.889670
## 669	NA 0.85885763	-7.041939e-02	GLU	16.889670
## 670	NA 0.71358663	7.527475e-01	GLU	16.889670
## 671	NA 0.89310289	-2.853611e-01	GLU	16.889670
## 672	NA 0.68659220	-6.368335e-02	GLU	16.889670
## 673	NA 0.52540249	3.978186e-01	GLU	16.889670
## 674	NA 0.87008229	9.670740e-03	GLU	16.889670
## 675	NA 0.72870219	1.344900e-01	GLU	16.889670
## 676	NA 0.40824707	-2.904395e-01	ALA	14.970386
## 677	NA 0.63544241	-1.042204e+00	ALA	14.970386
## 678	NA 0.09341622	-9.708903e-02	ALA	14.970386
## 679	NA 0.75314557	-4.622815e-01	ALA	14.970386
## 680	NA 0.13901093	-2.296183e-01	ALA	14.970386

## 681	1338576	0.59950985	-4.852134e-01	ALA	14.970386
## 682		NA 0.21028783	6.542201e-02	ALA	14.970386
## 683		NA 0.55783597	-7.097051e-01	ALA	14.970386
## 684		NA 0.38659792	-5.964792e-01	ALA	14.970386
## 685		NA 0.25141793	-1.650704e-01	ALA	14.970386
## 686		NA 0.49119076	1.335005e-01	ALA	14.970386
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## 688		NA 0.49181819	-1.101301e-01	ALA	14.970386
## 689		NA 0.74102556	-1.199365e-01	ALA	14.970386
## 690		NA 0.20242843	-3.189292e-02	ALA	14.970386
## 691		NA 0.48290435	-2.199149e-01	ALA	14.970386
## 692		NA 0.28480161	1.357919e-01	ALA	14.970386
## 693		NA 0.40944218	-1.845881e-01	ALA	14.970386
## 694		NA 0.81356257	-2.522667e-01	SER	12.355933
## 695		NA 0.83155233	-1.248871e-02	SER	12.355933
## 696		NA 0.84963934	-1.831960e-01	SER	12.355933
## 697		NA 0.76662108	-1.628896e-01	SER	12.355933
## 698		NA 0.41526129	6.070614e-03	SER	12.355933
## 699		NA 0.78575962	-2.109336e-01	SER	12.355933
## 700		NA 0.82082216	4.480576e-01	SER	12.355933
## 701		NA 0.64063469	2.231606e-01	SER	12.355933
## 702		NA 0.84703049	-6.646432e-01	SER	12.355933
## 703		NA 0.71271129	-5.669456e-01	SER	12.355933
## 704		NA 0.80118182	3.916106e-02	SER	12.355933
## 705		NA 0.74871764	-1.532239e-01	SER	12.355933
## 706		NA 0.73329276	7.076422e-01	SER	12.355933
## 707	3383913	0.65922361	8.792895e-02	SER	12.355933
## 708		NA 0.81075426	1.623189e+00	SER	12.355933
## 709		NA 0.85041022	2.851305e-01	SER	12.355933
## 710		NA 0.64577618	-2.820275e-01	SER	12.355933
## 711		NA 0.29706205	-9.139602e-03	SER	12.355933
## 712		NA 0.34349304	-3.384441e-01	VAL	11.132232
## 713		NA 0.82114100	-1.179185e-01	VAL	11.132232
## 714		NA 0.19977340	-3.503907e-01	VAL	11.132232
## 715		NA 0.24271033	-2.821164e-01	VAL	11.132232
## 716		NA 0.12643967	-4.392138e-01	VAL	11.132232
## 717		NA 0.14220390	-1.302855e-01	VAL	11.132232
## 718		NA 0.77190233	-1.292369e-01	VAL	11.132232
## 719		NA 0.85994397	-6.364466e-01	VAL	11.132232
## 720		NA 0.23074992	7.535923e-02	VAL	11.132232
## 721		NA 0.28881358	-2.767030e-01	VAL	11.132232
## 722		NA 0.11955790	-1.999827e-01	VAL	11.132232
## 723		NA 0.26222927	-2.840702e-02	VAL	11.132232
## 724		NA 0.14261552	-8.667054e-02	VAL	11.132232
## 725		NA 0.69144643	-3.153895e-01	VAL	11.132232
## 726		NA 0.29095959	-1.315582e-02	VAL	11.132232
## 727		NA 0.24930529	-2.060678e-01	VAL	11.132232
## 728		NA 0.79018280	-6.152808e-01	LYS	10.787749
## 729		NA 0.75827786	-1.939188e-01	LYS	10.787749
## 730		NA 0.82016911	8.508991e-01	LYS	10.787749
## 731		NA 0.80299751	5.567754e-02	LYS	10.787749
## 732		NA 0.45835466	-8.250640e-02	LYS	10.787749
## 733		NA 0.27144638	1.115687e-01	LYS	10.787749
## 734		NA 0.48314256	-6.920370e-02	LYS	10.787749

## 735	NA 0.69707554	2.629374e-01	LYS	10.787749
## 736	NA 0.73401849	3.349934e-02	LYS	10.787749
## 737	NA 0.50455345	-9.126728e-02	LYS	10.787749
## 738	NA 0.21876713	-3.559431e-02	LYS	10.787749
## 739	NA 0.52041741	-5.330972e-01	LYS	10.787749
## 740	NA 0.73538938	-7.258337e-01	LYS	10.787749
## 741	NA 0.36896054	-3.949884e-01	LYS	10.787749
## 742	NA 0.80292938	-6.306041e-01	LYS	10.787749
## 743	NA 0.76504776	-4.226274e-01	LYS	10.787749
## 744	NA 0.28880380	-2.382941e-01	LYS	10.787749
## 745	NA 0.41501108	-4.749716e-01	MET	11.146596
## 746	NA 0.59673704	-6.784368e-01	MET	11.146596
## 747	NA 0.16138957	-2.033060e-01	MET	11.146596
## 748	NA 0.25608247	-4.132762e-01	MET	11.146596
## 749	NA 0.34486163	-5.743116e-01	MET	11.146596
## 750	NA 0.11922962	4.187651e-02	MET	11.146596
## 751	NA 0.33421810	-2.156736e-01	MET	11.146596
## 752	NA 0.59808250	-5.065792e-01	MET	11.146596
## 753	NA 0.14431630	1.076360e+00	MET	11.146596
## 754	NA 0.09091293	6.501243e-02	MET	11.146596
## 755	NA 0.70490522	8.252232e-01	MET	11.146596
## 756	NA 0.46262246	-6.249745e-01	MET	11.146596
## 757	NA 0.10379092	1.297847e-01	MET	11.146596
## 758	NA 0.16334963	2.807376e-01	MET	11.146596
## 759	NA 0.43966580	-5.036295e-01	MET	11.146596
## 760	NA 0.24661927	-3.124681e-01	MET	11.146596
## 761	NA 0.28614448	9.297774e-02	MET	11.146596
## 762	NA 0.58274756	-4.941749e-01	MET	11.146596
## 763	NA 0.57911750	-7.057748e-01	LEU	10.012166
## 764	NA 0.76615347	-8.276698e-01	LEU	10.012166
## 765	NA 0.79748138	-9.441377e-01	LEU	10.012166
## 766	NA 0.08542366	-2.285310e-02	LEU	10.012166
## 767	NA 0.83940202	-7.882837e-01	LEU	10.012166
## 768	NA 0.80489337	-6.503157e-01	LEU	10.012166
## 769	NA 0.81585658	-3.223961e-01	LEU	10.012166
## 770	NA 0.86491797	-9.045866e-01	LEU	10.012166
## 771	NA 0.74199817	-4.629606e-01	LEU	10.012166
## 772	NA 0.79581893	-5.373617e-01	LEU	10.012166
## 773	NA 0.69154143	-8.127103e-01	LEU	10.012166
## 774	NA 0.55983810	-7.416459e-01	LEU	10.012166
## 775	NA 0.82974236	-4.956101e-01	LEU	10.012166
## 776	NA 0.79697393	8.366967e-01	LEU	10.012166
## 777	NA 0.72742784	-8.970970e-01	LEU	10.012166
## 778	NA 0.72495452	-1.017714e+00	LEU	10.012166
## 779	NA 0.95332692	-4.408190e-02	LEU	10.012166
## 780	NA 0.82667303	1.015969e+00	LEU	10.012166
## 781	NA 0.44911835	5.239938e-01	PRO	12.503146
## 782	NA 0.52778357	4.700173e-02	PRO	12.503146
## 783	NA 0.15043497	3.138550e-02	PRO	12.503146
## 784	NA 0.48217513	-4.522200e-01	PRO	12.503146
## 785	NA 0.69527386	-6.934911e-01	PRO	12.503146
## 786	NA 0.45693318	-8.635381e-01	PRO	12.503146
## 787	NA 0.20641256	-2.265065e-01	PRO	12.503146
## 788	NA 0.68020862	-7.158565e-01	PRO	12.503146

## 789	NA	0.33303349	-3.255724e-01	PRO	12.503146
## 790	NA	0.65783160	-8.795656e-01	PRO	12.503146
## 791	36205	0.70597334	-8.694310e-01	PRO	12.503146
## 792	NA	0.70281549	-9.458644e-01	PRO	12.503146
## 793	NA	0.11858240	-4.021760e-01	PRO	12.503146
## 794	NA	0.52184002	-2.910588e-01	PRO	12.503146
## 795	NA	0.72225759	-5.731027e-01	PRO	12.503146
## 796	NA	0.86562787	-1.003270e+00	PRO	12.503146
## 797	NA	0.75257366	-4.644196e-01	PRO	12.503146
## 798	NA	0.18337006	2.135497e-01	PRO	12.503146
## 799	NA	0.47781209	2.225765e-01	THR	11.507684
## 800	NA	0.85354446	5.524722e-02	THR	11.507684
## 801	NA	0.35140238	-3.621123e-01	THR	11.507684
## 802	NA	0.49166552	-4.510393e-01	THR	11.507684
## 803	NA	0.59996826	-7.880200e-01	THR	11.507684
## 804	NA	0.52283012	-7.039479e-01	THR	11.507684
## 805	NA	0.48391417	-6.651350e-01	THR	11.507684
## 806	NA	0.11108790	-6.828621e-03	THR	11.507684
## 807	NA	0.61477160	-6.685902e-01	THR	11.507684
## 808	NA	0.71974886	-6.634071e-01	THR	11.507684
## 809	NA	0.51971877	-5.117625e-01	THR	11.507684
## 810	NA	0.24750432	-3.673213e-01	THR	11.507684
## 811	NA	0.27706620	-2.593337e-01	THR	11.507684
## 812	NA	0.70914700	-6.137618e-02	THR	11.507684
## 813	NA	0.69752230	-3.373272e-01	THR	11.507684
## 814	NA	0.41846361	-6.501744e-01	THR	11.507684
## 815	NA	0.44615745	-5.746875e-01	THR	11.507684
## 816	NA	0.67448899	-8.031689e-01	TYR	15.198603
## 817	NA	0.81225710	-1.013477e+00	TYR	15.198603
## 818	NA	0.81646167	-4.880523e-01	TYR	15.198603
## 819	NA	0.74022024	-7.694337e-01	TYR	15.198603
## 820	NA	0.86652412	1.136925e-01	TYR	15.198603
## 821	NA	0.79138439	-8.161167e-01	TYR	15.198603
## 822	NA	0.72150476	-2.838953e-01	TYR	15.198603
## 823	NA	0.82437186	-8.974425e-01	TYR	15.198603
## 824	NA	0.58758576	-1.421064e-01	TYR	15.198603
## 825	NA	0.80632301	-7.930259e-01	TYR	15.198603
## 826	NA	0.54203682	-6.203005e-01	TYR	15.198603
## 827	NA	0.58606580	-5.543910e-01	TYR	15.198603
## 828	NA	0.71910478	-5.257818e-01	TYR	15.198603
## 829	NA	0.76097648	-1.133850e+00	TYR	15.198603
## 830	NA	0.63656150	-6.414882e-01	TYR	15.198603
## 831	NA	0.82103134	-6.296119e-01	TYR	15.198603
## 832	NA	0.43307284	-2.346281e-01	TYR	15.198603
## 833	NA	0.64717114	-5.578966e-01	TYR	15.198603
## 834	NA	0.80749887	-6.343240e-01	TYR	15.198603
## 835	585917	0.61150701	-4.429250e-01	VAL	15.109626
## 836	NA	0.84335398	-5.808992e-01	VAL	15.109626
## 837	NA	0.52103508	-3.991141e-01	VAL	15.109626
## 838	NA	0.74682329	-3.817039e-01	VAL	15.109626
## 839	NA	0.47354062	-5.423993e-01	VAL	15.109626
## 840	NA	0.81772402	-6.138482e-01	VAL	15.109626
## 841	NA	0.73053694	-8.403368e-02	VAL	15.109626
## 842	NA	0.14924801	-1.283297e-01	VAL	15.109626

## 843	NA	0.67980005	1.611468e+00	VAL	15.109626
## 844	419624	0.53949378	4.319710e-01	VAL	15.109626
## 845	NA	0.37347746	-3.813567e-01	VAL	15.109626
## 846	NA	0.36368234	-7.279833e-01	VAL	15.109626
## 847	NA	0.22857051	-1.460272e-02	VAL	15.109626
## 848	NA	0.38397337	-3.641551e-01	VAL	15.109626
## 849	NA	0.33503900	-2.586487e-01	VAL	15.109626
## 850	NA	0.29736543	-2.549365e-01	VAL	15.109626
## 851	NA	0.72838386	-5.457592e-01	VAL	15.109626
## 852	NA	0.66680462	4.404641e-01	VAL	15.109626
## 853	NA	0.84172031	1.672432e-01	ARG	18.238680
## 854	447391	0.85878488	3.852176e-01	ARG	18.238680
## 855	NA	0.84615545	8.251337e-01	ARG	18.238680
## 856	NA	0.81790515	1.196179e-01	ARG	18.238680
## 857	NA	0.78606898	8.090147e-01	ARG	18.238680
## 858	NA	0.74006489	1.513992e+00	ARG	18.238680
## 859	NA	0.81780136	2.062128e+00	ARG	18.238680
## 860	NA	0.16981957	9.368820e-01	ARG	18.238680
## 861	NA	0.40110403	1.451007e+00	ARG	18.238680
## 862	NA	0.85076872	7.868188e-01	ARG	18.238680
## 863	NA	0.77348391	9.975416e-01	ARG	18.238680
## 864	NA	0.76845366	2.830393e-01	ARG	18.238680
## 865	NA	0.66007557	4.699966e-01	ARG	18.238680
## 866	NA	0.81373255	1.002282e+00	ARG	18.238680
## 867	2779779	0.74695922	6.519519e-01	ARG	18.238680
## 868	NA	0.75073971	-5.106970e-01	ARG	18.238680
## 869	NA	0.77693210	7.017585e-01	ARG	18.238680
## 870	NA	0.77357135	-1.441353e-01	ARG	18.238680
## 871	NA	0.78407764	4.102140e-01	ARG	18.238680
## 872	NA	0.86970507	8.267371e-01	SER	20.004220
## 873	NA	0.83400534	1.005310e+00	SER	20.004220
## 874	NA	0.85854118	8.244895e-01	SER	20.004220
## 875	NA	0.86187276	3.616902e+00	SER	20.004220
## 876	NA	0.86276734	1.536062e+00	SER	20.004220
## 877	NA	0.80137727	1.859634e+00	SER	20.004220
## 878	NA	0.58123455	3.627023e+00	SER	20.004220
## 879	NA	0.84861146	-1.852845e-01	SER	20.004220
## 880	NA	0.65462327	3.212096e+00	SER	20.004220
## 881	NA	0.79797026	2.238749e+00	SER	20.004220
## 882	NA	0.91107622	1.463163e+00	SER	20.004220
## 883	NA	0.76989255	1.891998e+00	SER	20.004220
## 884	NA	0.83224059	2.144746e-01	SER	20.004220
## 885	NA	0.69834198	7.980370e-01	SER	20.004220
## 886	NA	0.83218529	1.232489e+00	SER	20.004220
## 887	NA	0.79824117	2.358752e+00	SER	20.004220
## 888	NA	0.82843838	1.638552e+00	SER	20.004220
## 889	NA	0.69415612	2.268284e+00	SER	20.004220
## 890	NA	0.71300637	1.049474e+00	THR	21.377225
## 891	NA	0.82863593	1.603623e+00	THR	21.377225
## 892	NA	0.34082812	1.049085e+00	THR	21.377225
## 893	NA	0.82932220	-4.967808e-01	THR	21.377225
## 894	NA	0.79256433	8.397395e-01	THR	21.377225
## 895	NA	0.69534372	1.208660e+00	THR	21.377225
## 896	NA	0.71903636	2.972082e-01	THR	21.377225

## 897	NA 0.66335850	9.132239e-01	THR	21.377225
## 898	NA 0.89072225	3.251296e+00	THR	21.377225
## 899	NA 0.80488988	2.814405e+00	THR	21.377225
## 900	NA 0.86175363	1.044024e+00	THR	21.377225
## 901	NA 0.66910071	1.535431e+00	THR	21.377225
## 902	NA 0.83389170	1.383383e+00	THR	21.377225
## 903	NA 0.79615992	2.844825e+00	THR	21.377225
## 904	NA 0.87313311	5.351061e-01	THR	21.377225
## 905	NA 0.88365911	-6.489317e-02	THR	21.377225
## 906	NA 0.82763940	1.982202e+00	THR	21.377225
## 907	NA 0.51661114	4.513347e-01	THR	21.377225
## 908	NA 0.91866298	9.789087e-01	PRO	23.786699
## 909	NA 0.63486807	2.087373e+00	PRO	23.786699
## 910	NA 0.77243184	-3.250096e-01	PRO	23.786699
## 911	NA 0.45843855	6.558328e-01	PRO	23.786699
## 912	NA 0.76141362	1.202942e+00	PRO	23.786699
## 913	NA 0.78950779	-4.407438e-01	PRO	23.786699
## 914	NA 0.81388117	8.264636e-02	PRO	23.786699
## 915	NA 0.68169251	-3.303398e-01	PRO	23.786699
## 916	NA 0.79408119	9.072160e-01	PRO	23.786699
## 917	NA 0.73876875	4.270747e-01	PRO	23.786699
## 918	NA 0.75730314	9.028141e-01	PRO	23.786699
## 919	NA 0.57461978	6.723912e-01	PRO	23.786699
## 920	NA 0.80453074	4.688223e-01	PRO	23.786699
## 921	NA 0.76798845	3.615780e-01	PRO	23.786699
## 922	NA 0.47215695	6.533166e-01	PRO	23.786699
## 923	NA 0.81584931	4.080378e-01	PRO	23.786699
## 924	NA 0.82827371	6.331577e-01	PRO	23.786699
## 925	NA 0.68069138	1.034666e+00	PRO	23.786699
## 926	NA 0.75105945	1.825221e+00	GLU	25.814973
## 927	NA 0.82791907	1.721895e+00	GLU	25.814973
## 928	NA 0.90683638	1.894004e+00	GLU	25.814973
## 929	NA 0.85741692	-1.885008e-01	GLU	25.814973
## 930	NA 0.76076713	4.560344e-02	GLU	25.814973
## 931	NA 0.71613998	2.608293e-01	GLU	25.814973
## 932	NA 0.73809674	2.162553e+00	GLU	25.814973
## 933	NA 0.42935154	2.105702e+00	GLU	25.814973
## 934	NA 0.63520694	-5.452734e-01	GLU	25.814973
## 935	NA 0.77605051	1.184397e+00	GLU	25.814973
## 936	NA 0.76819637	3.773311e-01	GLU	25.814973
## 937	NA 0.78681116	1.278660e+00	GLU	25.814973
## 938	NA 0.76198890	-1.558654e-01	GLU	25.814973
## 939	NA 0.76347541	1.894431e+00	GLU	25.814973
## 940	NA 0.71388906	9.657169e-01	GLU	25.814973
## 941	NA 0.65442994	3.338845e-01	GLU	25.814973
## 942	NA 0.82495542	1.488462e+00	GLU	25.814973
## 943	NA 0.76897098	-2.884162e-01	GLU	25.814973
## 944	NA 0.79306137	-5.975529e-01	GLU	25.814973
## 945	NA 0.79839363	4.432227e-01	GLY	26.928652
## 946	NA 0.83270615	-1.159519e-01	GLY	26.928652
## 947	NA 1.00007914	1.603684e+00	GLY	26.928652
## 948	NA 0.76922489	7.030558e-01	GLY	26.928652
## 949	NA 0.80767487	1.100877e+00	GLY	26.928652
## 950	NA 0.78943275	1.282945e+00	GLY	26.928652

## 951	NA 0.75310673	1.939411e+00	GLY	26.928652
## 952	NA 0.73557630	-6.077976e-01	GLY	26.928652
## 953	NA 0.76466442	1.734694e+00	GLY	26.928652
## 954	NA 0.87195124	8.017093e-01	GLY	26.928652
## 955	NA 0.78576296	7.805217e-01	GLY	26.928652
## 956	NA 0.78824892	7.047483e-02	GLY	26.928652
## 957	NA 0.64337588	1.147204e+00	GLY	26.928652
## 958	NA 0.82274545	5.446356e-01	GLY	26.928652
## 959	NA 0.82622011	-5.333713e-01	GLY	26.928652
## 960	NA 0.72919506	9.341184e-01	GLY	26.928652
## 961	NA 0.75573137	6.409628e-02	GLY	26.928652
## 962	NA 0.86728930	4.170334e-01	GLY	26.928652
## 963	NA 0.78473455	6.494345e-02	SER	25.264893
## 964	NA 0.70373381	5.888024e-02	SER	25.264893
## 965	NA 0.85760608	3.464002e-01	SER	25.264893
## 966	NA 0.50473080	4.925884e-01	SER	25.264893
## 967	NA 0.73672643	3.721624e-01	SER	25.264893
## 968	NA 0.79296517	9.408050e-01	SER	25.264893
## 969	NA 0.82479475	5.830449e-01	SER	25.264893
## 970	NA 0.82300006	-2.994957e-01	SER	25.264893
## 971	NA 0.72204837	1.715251e+00	SER	25.264893
## 972	NA 0.81312567	-1.599032e-01	SER	25.264893
## 973	NA 0.87541997	-4.729450e-01	SER	25.264893
## 974	NA 0.84246952	1.934246e+00	SER	25.264893
## 975	NA 0.83648520	3.643145e-01	SER	25.264893
## 976	NA 0.51094848	-5.439719e-01	SER	25.264893
## 977	NA 0.70008485	1.553870e+00	SER	25.264893
## 978	NA 0.78009306	2.113343e+00	SER	25.264893
## 979	NA 0.80850727	4.972633e-01	SER	25.264893
## 980	NA 0.83015685	8.118688e-01	SER	25.264893
## 981	NA 0.84143649	3.944238e-02	SER	25.264893
## 982	NA 0.66840994	1.391306e+00	GLU	26.519582
## 983	NA 0.70881201	6.674244e-01	GLU	26.519582
## 984	NA 0.82635404	-4.063820e-01	GLU	26.519582
## 985	NA 0.81101880	-3.763461e-02	GLU	26.519582
## 986	NA 0.95830676	4.089010e-01	GLU	26.519582
## 987	NA 0.70941648	1.126991e+00	GLU	26.519582
## 988	NA 0.82570834	-3.780790e-01	GLU	26.519582
## 989	NA 0.61599926	1.041786e-01	GLU	26.519582
## 990	NA 0.77644109	-4.711241e-01	GLU	26.519582
## 991	NA 0.80392952	2.659041e-02	GLU	26.519582
## 992	NA 0.85357567	-4.243295e-01	GLU	26.519582
## 993	NA 0.72609517	6.646295e-02	GLU	26.519582
## 994	NA 0.60485750	-2.036761e-01	GLU	26.519582
## 995	NA 0.42656324	9.024689e-01	GLU	26.519582
## 996	NA 0.67610761	2.277014e+00	GLU	26.519582
## 997	NA 0.72974859	1.610294e+00	GLU	26.519582
## 998	NA 0.93499764	-2.856600e-01	GLU	26.519582
## 999	NA 0.87725557	-1.405586e-01	GLU	26.519582
## 1000	NA 0.82608565	1.915698e+00	VAL	26.978056
## 1001	NA 0.85684944	1.718690e+00	VAL	26.978056
## 1002	NA 0.26709605	2.251122e+00	VAL	26.978056
## 1003	NA 0.81290429	1.379352e+00	VAL	26.978056
## 1004	NA 0.66850841	1.405760e+00	VAL	26.978056

## 1005	NA	0.76653210	1.747362e+00	VAL	26.978056
## 1006	NA	0.45735921	1.729331e+00	VAL	26.978056
## 1007	NA	0.62244696	2.256581e+00	VAL	26.978056
## 1008	NA	0.71964984	2.463077e-01	VAL	26.978056
## 1009	NA	0.87872001	6.099583e-01	VAL	26.978056
## 1010	NA	0.89693873	1.459502e+00	VAL	26.978056
## 1011	NA	0.53947675	1.789268e+00	VAL	26.978056
## 1012	NA	1.05099150	1.514663e+00	VAL	26.978056
## 1013	NA	0.77709338	2.725724e+00	VAL	26.978056
## 1014	NA	0.73428770	2.305940e+00	VAL	26.978056
## 1015	NA	0.76769459	2.501615e-01	VAL	26.978056
## 1016	NA	0.42604806	1.735445e+00	VAL	26.978056
## 1017	NA	0.48934182	6.432154e-01	VAL	26.978056
## 1018	NA	0.16448554	1.713441e-01	GLY	27.074975
## 1019	NA	0.57086470	-2.554978e-01	GLY	27.074975
## 1020	NA	0.49772218	-6.556140e-01	GLY	27.074975
## 1021	NA	0.33985627	-1.568041e-02	GLY	27.074975
## 1022	NA	0.25986904	-3.387789e-01	GLY	27.074975
## 1023	NA	0.37433539	-1.090404e-01	GLY	27.074975
## 1024	NA	0.43027167	-5.603858e-01	GLY	27.074975
## 1025	NA	0.38207627	-3.966157e-01	GLY	27.074975
## 1026	NA	0.48223495	-4.496776e-01	GLY	27.074975
## 1027	NA	0.13685827	5.419771e-01	GLY	27.074975
## 1028	NA	0.29766888	-4.775995e-01	GLY	27.074975
## 1029	NA	0.67488625	-6.417372e-01	GLY	27.074975
## 1030	NA	0.39898056	-1.490024e-01	GLY	27.074975
## 1031	36209	0.27686268	-8.584601e-02	GLY	27.074975
## 1032	NA	0.46262868	-9.641466e-01	GLY	27.074975
## 1033	NA	0.64637045	-4.540955e-01	GLY	27.074975
## 1034	NA	0.82239392	-4.259087e-01	GLY	27.074975
## 1035	NA	0.73162234	-1.188747e-01	GLY	27.074975
## 1036	NA	0.27845178	-2.204392e-02	ASP	25.172773
## 1037	NA	0.49097958	1.172733e+00	ASP	25.172773
## 1038	NA	0.69655701	2.244780e+00	ASP	25.172773
## 1039	NA	0.22430757	2.086949e+00	ASP	25.172773
## 1040	NA	0.49260258	-2.145151e-01	ASP	25.172773
## 1041	NA	0.35852072	8.717133e-01	ASP	25.172773
## 1042	NA	0.33294456	1.850506e+00	ASP	25.172773
## 1043	NA	0.50131880	-1.293588e-01	ASP	25.172773
## 1044	NA	0.51210445	2.334615e+00	ASP	25.172773
## 1045	NA	0.65566108	1.807833e+00	ASP	25.172773
## 1046	NA	0.31939349	4.094116e-01	ASP	25.172773
## 1047	NA	0.47681819	4.389203e-01	ASP	25.172773
## 1048	NA	0.26757242	4.011541e-01	ASP	25.172773
## 1049	NA	0.28275031	1.550264e+00	ASP	25.172773
## 1050	NA	0.40370356	3.723558e-02	ASP	25.172773
## 1051	NA	0.51078915	1.663580e+00	ASP	25.172773
## 1052	NA	0.68975563	1.259183e+00	ASP	25.172773
## 1053	NA	0.68204324	8.785924e-02	ASP	25.172773
## 1054	NA	0.26144206	3.277397e-01	ASP	25.172773
## 1055	NA	0.29341886	7.160521e-01	PHE	21.975363
## 1056	NA	0.87319055	1.123806e+00	PHE	21.975363
## 1057	NA	0.82365269	-7.058959e-02	PHE	21.975363
## 1058	NA	0.81424742	-5.532338e-01	PHE	21.975363

## 1059	NA 0.65531819	-2.658231e-01	PHE	21.975363
## 1060	NA 0.69460469	-1.590382e-01	PHE	21.975363
## 1061	NA 0.80123688	2.669165e-01	PHE	21.975363
## 1062	NA 0.27499287	-4.828529e-01	PHE	21.975363
## 1063	NA 0.82158858	-3.211906e-01	PHE	21.975363
## 1064	NA 0.55886538	-2.095208e-01	PHE	21.975363
## 1065	NA 0.28832613	1.621351e+00	PHE	21.975363
## 1066	NA 0.49067176	-5.017505e-01	PHE	21.975363
## 1067	NA 0.69405755	-3.479812e-01	PHE	21.975363
## 1068	NA 0.23408381	-3.900363e-01	PHE	21.975363
## 1069	NA 0.85118506	-4.375461e-01	PHE	21.975363
## 1070	NA 0.65618092	-7.076063e-01	PHE	21.975363
## 1071	NA 0.52151985	-3.264027e-01	PHE	21.975363
## 1072	NA 0.31956839	-2.027880e-02	PHE	21.975363
## 1073	NA 0.76390041	-7.411615e-02	PHE	21.975363
## 1074	NA 0.48493855	-5.782109e-01	LEU	19.918086
## 1075	NA 0.51597061	1.067819e+00	LEU	19.918086
## 1076	NA 0.25201583	9.740479e-02	LEU	19.918086
## 1077	NA 0.52164190	-3.306056e-02	LEU	19.918086
## 1078	NA 0.34611433	-4.233637e-01	LEU	19.918086
## 1079	NA 0.58520267	1.317122e+00	LEU	19.918086
## 1080	NA 0.75948386	9.715430e-01	LEU	19.918086
## 1081	NA 0.32757557	3.331703e-01	LEU	19.918086
## 1082	NA 0.65339210	-4.459296e-01	LEU	19.918086
## 1083	NA 0.34204448	2.182667e-01	LEU	19.918086
## 1084	NA 0.43086382	2.891152e-01	LEU	19.918086
## 1085	NA 0.74292435	4.394181e-01	LEU	19.918086
## 1086	NA 0.21884641	-3.358938e-01	LEU	19.918086
## 1087	NA 0.38477745	-3.421545e-01	LEU	19.918086
## 1088	NA 0.64364817	3.668263e-01	LEU	19.918086
## 1089	NA 0.30952094	-3.936743e-01	LEU	19.918086
## 1090	NA 0.45070090	-3.472357e-01	LEU	19.918086
## 1091	NA 0.51902297	-5.699681e-01	LEU	19.918086
## 1092	NA 0.55063743	1.801102e-01	LEU	19.918086
## 1093	NA 0.75927425	1.333477e-01	SER	16.120787
## 1094	NA 0.65416503	-5.788927e-01	SER	16.120787
## 1095	NA 0.63935134	-6.149691e-01	SER	16.120787
## 1096	NA 0.77813779	-7.841556e-01	SER	16.120787
## 1097	NA 0.72553926	-7.503495e-01	SER	16.120787
## 1098	NA 0.80320628	1.712247e+00	SER	16.120787
## 1099	NA 0.68638046	-6.203068e-01	SER	16.120787
## 1100	NA 0.70962135	-6.957072e-01	SER	16.120787
## 1101	NA 0.58127542	-5.405497e-01	SER	16.120787
## 1102	NA 0.68717509	-9.492059e-01	SER	16.120787
## 1103	NA 0.79247351	-8.913089e-01	SER	16.120787
## 1104	NA 0.64198142	-5.904054e-01	SER	16.120787
## 1105	NA 0.72134419	-6.565982e-01	SER	16.120787
## 1106	NA 0.65868516	-5.842820e-01	SER	16.120787
## 1107	NA 0.66647437	-6.608111e-01	SER	16.120787
## 1108	NA 0.81911393	-7.758374e-01	SER	16.120787
## 1109	NA 0.64773959	-4.970143e-01	SER	16.120787
## 1110	NA 0.75373891	-7.060542e-01	SER	16.120787
## 1111	NA 0.67639563	-5.504571e-01	LEU	14.120302
## 1112	NA 0.72702520	-5.333077e-01	LEU	14.120302

## 1113	NA 0.79102546	-8.062509e-01	LEU	14.120302
## 1114	NA 0.88019167	-9.588244e-01	LEU	14.120302
## 1115	NA 0.69910072	-8.461256e-01	LEU	14.120302
## 1116	NA 0.46002354	-4.002839e-02	LEU	14.120302
## 1117	NA 0.63121179	-6.708943e-01	LEU	14.120302
## 1118	NA 0.71225897	-6.967837e-01	LEU	14.120302
## 1119	NA 0.51463274	-7.684628e-01	LEU	14.120302
## 1120	NA 0.28293261	-4.079901e-01	LEU	14.120302
## 1121	NA 0.29171008	-4.349475e-01	LEU	14.120302
## 1122	NA 0.87575519	-6.350671e-01	LEU	14.120302
## 1123	NA 0.56718207	-5.634383e-01	LEU	14.120302
## 1124	NA 0.81246913	-6.408037e-01	LEU	14.120302
## 1125	NA 0.78239477	-9.250598e-01	LEU	14.120302
## 1126	NA 0.60529637	-8.321947e-01	LEU	14.120302
## 1127	NA 0.75091835	-8.884833e-01	LEU	14.120302
## 1128	NA 0.75566768	-7.384439e-01	LEU	14.120302
## 1129	NA 0.29284084	-3.146829e-01	LEU	14.120302
## 1130	NA 0.74433040	-7.407673e-01	VAL	16.452176
## 1131	NA 0.76412510	-8.092564e-01	VAL	16.452176
## 1132	NA 0.51993973	-1.286477e-01	VAL	16.452176
## 1133	NA 0.65893552	-8.272638e-01	VAL	16.452176
## 1134	NA 0.69782758	-3.300005e-01	VAL	16.452176
## 1135	NA 0.69152113	-6.402878e-01	VAL	16.452176
## 1136	NA 0.15439910	-2.638855e-01	VAL	16.452176
## 1137	NA 0.60948127	2.243077e-01	VAL	16.452176
## 1138	NA 0.67094661	-9.412841e-01	VAL	16.452176
## 1139	NA 0.77511414	-5.870191e-01	VAL	16.452176
## 1140	NA 0.70513827	-6.606388e-01	VAL	16.452176
## 1141	NA 0.74526703	-8.624223e-01	VAL	16.452176
## 1142	NA 0.58161724	-5.061996e-01	VAL	16.452176
## 1143	NA 0.68380033	-8.442431e-01	VAL	16.452176
## 1144	NA 0.39528258	-4.990521e-01	VAL	16.452176
## 1145	NA 0.76030490	-9.024697e-01	VAL	16.452176
## 1146	NA 0.73692288	-4.162431e-01	VAL	16.452176
## 1147	NA 0.52525626	-6.888276e-01	VAL	16.452176
## 1148	NA 0.71615751	-6.932321e-01	VAL	16.452176
## 1149	NA 0.84918810	1.774513e+00	MET	18.092327
## 1150	NA 0.82059484	-4.795804e-01	MET	18.092327
## 1151	NA 0.92048434	-1.045456e+00	MET	18.092327
## 1152	NA 0.71670701	5.756177e-03	MET	18.092327
## 1153	NA 0.79359794	1.594076e-01	MET	18.092327
## 1154	NA 0.61419806	-7.429754e-01	MET	18.092327
## 1155	NA 0.68936215	-6.240323e-01	MET	18.092327
## 1156	NA 0.73233520	1.116420e+00	MET	18.092327
## 1157	NA 0.60880015	-2.940183e-01	MET	18.092327
## 1158	NA 0.66288771	-1.957822e-01	MET	18.092327
## 1159	NA 0.58111981	1.106093e-01	MET	18.092327
## 1160	NA 0.67201318	-3.775565e-01	MET	18.092327
## 1161	NA 0.68936114	-1.076611e+00	MET	18.092327
## 1162	NA 0.70237786	-3.409532e-01	MET	18.092327
## 1163	NA 0.67551150	1.549633e+00	MET	18.092327
## 1164	NA 0.65544058	-1.341635e-01	MET	18.092327
## 1165	NA 0.84478398	-4.320813e-01	MET	18.092327
## 1166	NA 0.82563613	-8.337374e-01	MET	18.092327

## 1167	NA 0.53547584	5.984354e-01	LEU	20.822593
## 1168	NA 0.69002788	-1.629300e-01	LEU	20.822593
## 1169	NA 0.62128316	-8.070245e-01	LEU	20.822593
## 1170	NA 0.79072923	-6.686452e-01	LEU	20.822593
## 1171	NA 0.61782972	-1.751435e-01	LEU	20.822593
## 1172	NA 0.69233441	1.408369e+00	LEU	20.822593
## 1173	NA 0.73157692	-7.008842e-01	LEU	20.822593
## 1174	NA 0.61796902	-1.874341e-01	LEU	20.822593
## 1175	NA 0.77477459	-1.179849e-01	LEU	20.822593
## 1176	NA 0.78721900	6.245163e-02	LEU	20.822593
## 1177	NA 0.74370292	-4.134399e-01	LEU	20.822593
## 1178	NA 0.78802685	-2.145882e-02	LEU	20.822593
## 1179	NA 0.71815798	-3.870942e-01	LEU	20.822593
## 1180	NA 0.81194611	1.065602e+00	LEU	20.822593
## 1181	NA 0.46323272	-4.684684e-01	LEU	20.822593
## 1182	NA 0.81286291	-5.478948e-01	LEU	20.822593
## 1183	NA 0.54363873	1.892643e-01	LEU	20.822593
## 1184	NA 0.84928068	1.705277e-01	LEU	20.822593
## 1185	NA 0.75400246	5.994008e-01	VAL	20.742386
## 1186	NA 0.65166163	1.316929e+00	VAL	20.742386
## 1187	NA 0.28248536	-3.538514e-01	VAL	20.742386
## 1188	NA 0.73326515	-3.978897e-01	VAL	20.742386
## 1189	NA 0.48463199	-6.578607e-01	VAL	20.742386
## 1190	NA 0.68781806	-8.077337e-01	VAL	20.742386
## 1191	NA 0.86521621	-6.097341e-01	VAL	20.742386
## 1192	NA 0.44077925	-3.416119e-01	VAL	20.742386
## 1193	NA 0.74552448	1.487407e+00	VAL	20.742386
## 1194	NA 0.67522124	4.984237e-01	VAL	20.742386
## 1195	NA 0.72377664	-4.935623e-01	VAL	20.742386
## 1196	NA 0.30766196	-5.738148e-01	VAL	20.742386
## 1197	NA 0.47075263	-4.064056e-01	VAL	20.742386
## 1198	NA 0.31252368	-1.139089e-01	VAL	20.742386
## 1199	NA 0.64208223	-1.044048e-02	VAL	20.742386
## 1200	NA 0.74750211	9.307363e-02	VAL	20.742386
## 1201	NA 0.53254977	-5.781149e-01	VAL	20.742386
## 1202	NA 0.56935160	-7.418393e-01	VAL	20.742386
## 1203	NA 0.71625255	1.315706e+00	LYS	23.899200
## 1204	NA 0.77188074	5.858330e-01	LYS	23.899200
## 1205	NA 0.64262565	1.900584e+00	LYS	23.899200
## 1206	NA 0.60936704	-4.065181e-01	LYS	23.899200
## 1207	NA 0.77904602	3.881058e-01	LYS	23.899200
## 1208	NA 0.66994172	1.917379e+00	LYS	23.899200
## 1209	NA 0.73994379	2.159086e-01	LYS	23.899200
## 1210	NA 0.69454884	1.685288e-01	LYS	23.899200
## 1211	NA 0.74861215	5.305637e-01	LYS	23.899200
## 1212	NA 0.79651326	1.897308e+00	LYS	23.899200
## 1213	NA 0.76486886	1.078929e+00	LYS	23.899200
## 1214	NA 0.77544199	6.029429e-01	LYS	23.899200
## 1215	NA 0.78048312	-6.427791e-01	LYS	23.899200
## 1216	NA 0.67870659	6.051308e-01	LYS	23.899200
## 1217	NA 0.81518157	1.487428e+00	LYS	23.899200
## 1218	NA 0.67863329	-1.126245e-01	LYS	23.899200
## 1219	NA 0.76919850	8.070692e-01	LYS	23.899200
## 1220	NA 0.75263685	1.855602e+00	LYS	23.899200

## 1221	NA 0.49891354	-5.930169e-01	LYS	23.899200
## 1222	NA 0.79831238	1.385388e-01	VAL	23.760417
## 1223	NA 0.89287165	-4.016241e-01	VAL	23.760417
## 1224	NA 0.57998042	-6.164038e-01	VAL	23.760417
## 1225	NA 0.71802728	-6.854679e-01	VAL	23.760417
## 1226	NA 0.81504571	6.999892e-01	VAL	23.760417
## 1227	NA 0.73655275	-5.494450e-01	VAL	23.760417
## 1228	NA 0.74141978	-8.657366e-01	VAL	23.760417
## 1229	NA 0.82150373	1.236284e+00	VAL	23.760417
## 1230	NA 0.55918600	3.256566e-01	VAL	23.760417
## 1231	NA 0.82636399	2.220945e+00	VAL	23.760417
## 1232	NA 0.81991424	3.760938e-01	VAL	23.760417
## 1233	NA 0.69270260	-6.247480e-01	VAL	23.760417
## 1234	NA 0.50600719	-2.487784e-01	VAL	23.760417
## 1235	NA 0.71957119	-2.952001e-01	VAL	23.760417
## 1236	NA 0.56118298	1.388482e-01	VAL	23.760417
## 1237	NA 0.82747735	-3.839888e-01	VAL	23.760417
## 1238	NA 0.81734971	-3.597609e-01	VAL	23.760417
## 1239	NA 0.55854128	-4.201844e-01	VAL	23.760417
## 1240	NA 0.64622281	-1.328289e-01	VAL	23.760417
## 1241	NA 0.83523976	-7.904587e-01	GLY	26.839594
## 1242	NA 0.87733824	-1.049483e-01	GLY	26.839594
## 1243	NA 0.74661718	5.722621e-02	GLY	26.839594
## 1244	NA 0.75046340	8.126502e-01	GLY	26.839594
## 1245	NA 0.78545618	-4.489571e-01	GLY	26.839594
## 1246	NA 0.78331982	-7.360645e-01	GLY	26.839594
## 1247	NA 0.78431322	-3.732360e-01	GLY	26.839594
## 1248	NA 0.75554094	-7.358797e-01	GLY	26.839594
## 1249	NA 0.68486035	-4.431491e-01	GLY	26.839594
## 1250	NA 0.73317533	8.188465e-01	GLY	26.839594
## 1251	NA 0.78965172	2.291413e-01	GLY	26.839594
## 1252	NA 0.43589306	5.732983e-01	GLY	26.839594
## 1253	NA 0.85399148	-1.684418e-01	GLY	26.839594
## 1254	NA 0.63458885	-1.200229e-01	GLY	26.839594
## 1255	NA 0.79470979	-4.343471e-01	GLY	26.839594
## 1256	NA 0.85639270	-6.635470e-01	GLY	26.839594
## 1257	NA 0.73656172	-3.879036e-01	GLY	26.839594
## 1258	NA 0.74523625	2.442572e-01	GLY	26.839594
## 1259	NA 0.75613382	-3.949610e-01	GLU	28.218407
## 1260	NA 0.82482270	1.618646e-01	GLU	28.218407
## 1261	NA 0.84176069	-4.852871e-01	GLU	28.218407
## 1262	NA 0.84659380	-9.088207e-02	GLU	28.218407
## 1263	NA 0.88338962	3.192771e-01	GLU	28.218407
## 1264	NA 0.86980084	-2.443925e-01	GLU	28.218407
## 1265	NA 0.90111860	-1.029635e+00	GLU	28.218407
## 1266	NA 0.82884617	2.095516e-01	GLU	28.218407
## 1267	NA 0.81496594	-1.637997e-01	GLU	28.218407
## 1268	NA 0.84610264	-4.088802e-01	GLU	28.218407
## 1269	NA 0.82313615	-3.717125e-01	GLU	28.218407
## 1270	NA 0.74795825	-3.330376e-01	GLU	28.218407
## 1271	NA 0.79377186	-2.451185e-01	GLU	28.218407
## 1272	NA 0.80157378	3.065233e-01	GLU	28.218407
## 1273	NA 0.77307089	-2.191069e-01	GLU	28.218407
## 1274	NA 0.81662555	1.335352e+00	GLU	28.218407

## 1275	NA 0.85567777	-3.019287e-01	GLU	28.218407
## 1276	NA 0.73346069	-2.619229e-02	GLU	28.218407
## 1277	NA 0.88706360	9.719695e-01	GLU	28.218407
## 1278	NA 0.75285629	2.914660e-01	GLY	28.352156
## 1279	NA 0.78727730	-6.196314e-01	GLY	28.352156
## 1280	NA 0.79877556	-5.111699e-02	GLY	28.352156
## 1281	NA 0.81983334	-3.209800e-01	GLY	28.352156
## 1282	NA 0.72027468	5.342143e-01	GLY	28.352156
## 1283	NA 0.51886486	1.126628e+00	GLY	28.352156
## 1284	NA 0.79104178	5.615668e-01	GLY	28.352156
## 1285	NA 0.72273448	-1.351902e-03	GLY	28.352156
## 1286	NA 0.75552969	4.038842e-01	GLY	28.352156
## 1287	NA 0.67065640	6.940064e-01	GLY	28.352156
## 1288	NA 0.70940372	1.619431e-01	GLY	28.352156
## 1289	NA 0.83340336	-1.017027e-01	GLY	28.352156
## 1290	NA 0.78523383	5.132748e-01	GLY	28.352156
## 1291	NA 0.67026305	1.669345e+00	GLY	28.352156
## 1292	NA 0.80230618	2.256660e-01	GLY	28.352156
## 1293	NA 0.72409841	-7.124181e-02	GLY	28.352156
## 1294	NA 0.82846411	-1.604086e-01	GLY	28.352156
## 1295	NA 0.54845365	-7.799459e-01	GLY	28.352156
## 1296	NA 0.71715306	-3.500249e-01	GLU	29.881392
## 1297	NA 0.85513089	3.180187e-02	GLU	29.881392
## 1298	NA 0.82932841	1.754058e-01	GLU	29.881392
## 1299	NA 0.75819678	1.755906e-01	GLU	29.881392
## 1300	NA 0.79816822	2.614956e-01	GLU	29.881392
## 1301	NA 0.86669917	-1.866890e-01	GLU	29.881392
## 1302	NA 0.68926519	2.192285e-01	GLU	29.881392
## 1303	NA 0.82592905	2.862197e-02	GLU	29.881392
## 1304	NA 0.73794894	-7.731969e-02	GLU	29.881392
## 1305	NA 0.72396242	5.794988e-02	GLU	29.881392
## 1306	NA 0.89982366	-1.609446e-01	GLU	29.881392
## 1307	NA 0.83490664	5.016979e-02	GLU	29.881392
## 1308	NA 0.59379167	-1.540276e-01	GLU	29.881392
## 1309	NA 0.82669898	3.183301e-01	GLU	29.881392
## 1310	NA 0.77193581	-1.304736e-01	GLU	29.881392
## 1311	NA 0.83767263	3.751336e-01	GLU	29.881392
## 1312	NA 0.69960515	6.094737e-01	GLU	29.881392
## 1313	NA 0.86136813	-1.093403e-01	GLU	29.881392
## 1314	NA 0.82739301	-2.240938e-01	GLU	29.881392
## 1315	NA 0.84472433	2.268068e-01	GLU	26.957435
## 1316	NA 0.84819411	3.729831e-01	GLU	26.957435
## 1317	NA 0.70556245	2.697068e-01	GLU	26.957435
## 1318	NA 0.63341173	1.029153e+00	GLU	26.957435
## 1319	NA 0.78930120	-3.297192e-01	GLU	26.957435
## 1320	NA 0.82102486	2.468632e-01	GLU	26.957435
## 1321	NA 0.83248647	2.133673e-01	GLU	26.957435
## 1322	NA 0.77179755	3.317892e-01	GLU	26.957435
## 1323	NA 0.78860402	-4.549119e-01	GLU	26.957435
## 1324	NA 0.88159182	-8.444705e-03	GLU	26.957435
## 1325	NA 0.83263418	-1.304057e-01	GLU	26.957435
## 1326	NA 0.87137788	-6.570779e-01	GLU	26.957435
## 1327	NA 0.80514815	2.910526e-01	GLU	26.957435
## 1328	NA 0.83715032	3.256138e-01	GLU	26.957435

## 1329	NA 0.84450522	3.032180e-01	GLU	26.957435
## 1330	NA 0.81024106	1.625484e-01	GLU	26.957435
## 1331	NA 0.81129226	4.090103e-01	GLU	26.957435
## 1332	NA 0.81824022	-9.449242e-02	GLU	26.957435
## 1333	NA 0.80159414	8.841786e-01	GLU	26.957435
## 1334	NA 0.72628552	4.771057e-01	GLY	25.408297
## 1335	NA 0.72010986	4.444984e-01	GLY	25.408297
## 1336	NA 0.79117416	3.744277e-01	GLY	25.408297
## 1337	NA 0.74215732	6.139632e-01	GLY	25.408297
## 1338	NA 0.81131195	2.521846e+00	GLY	25.408297
## 1339	NA 0.80666308	-3.498139e-01	GLY	25.408297
## 1340	NA 0.77065740	5.961999e-01	GLY	25.408297
## 1341	NA 0.65638436	5.427850e-01	GLY	25.408297
## 1342	NA 0.73063806	-7.129766e-01	GLY	25.408297
## 1343	NA 0.91502017	7.167632e-01	GLY	25.408297
## 1344	NA 0.64320016	-7.224237e-02	GLY	25.408297
## 1345	NA 0.62214251	6.293151e-01	GLY	25.408297
## 1346	NA 0.86794579	4.459126e-01	GLY	25.408297
## 1347	NA 0.56557729	3.332553e-01	GLY	25.408297
## 1348	NA 0.85314022	-2.802378e-01	GLY	25.408297
## 1349	NA 0.73688813	4.513823e-01	GLY	25.408297
## 1350	NA 0.87735880	-4.407505e-01	GLY	25.408297
## 1351	NA 0.76770113	3.375231e-01	GLY	25.408297
## 1352	NA 0.45235635	7.494775e-01	GLN	24.263518
## 1353	NA 0.82585527	-7.908841e-02	GLN	24.263518
## 1354	NA 0.72324209	-1.356536e-01	GLN	24.263518
## 1355	NA 0.77182759	-6.672094e-02	GLN	24.263518
## 1356	NA 0.83659590	3.826745e-01	GLN	24.263518
## 1357	NA 0.79254964	4.948874e-01	GLN	24.263518
## 1358	NA 0.68731618	-1.424310e-01	GLN	24.263518
## 1359	NA 0.77903448	-7.305566e-01	GLN	24.263518
## 1360	NA 0.87369227	5.242893e-01	GLN	24.263518
## 1361	NA 0.79432133	6.006797e-01	GLN	24.263518
## 1362	NA 0.79416227	-7.321110e-01	GLN	24.263518
## 1363	NA 0.74907770	5.347296e-01	GLN	24.263518
## 1364	NA 0.69448823	3.045924e-02	GLN	24.263518
## 1365	NA 0.80133379	-3.282299e-01	GLN	24.263518
## 1366	NA 0.80074162	7.953712e-02	GLN	24.263518
## 1367	NA 0.65091869	-4.530199e-01	GLN	24.263518
## 1368	NA 0.85195336	3.583513e-01	GLN	24.263518
## 1369	NA 0.78872103	3.798030e-01	GLN	24.263518
## 1370	NA 0.82183011	-4.444590e-01	GLN	24.263518
## 1371	NA 0.76806511	2.257825e+00	TRP	23.880425
## 1372	NA 0.70631344	1.513635e+00	TRP	23.880425
## 1373	NA 0.69004779	6.516843e-01	TRP	23.880425
## 1374	NA 0.66934085	6.711819e-01	TRP	23.880425
## 1375	NA 0.79842440	8.156869e-01	TRP	23.880425
## 1376	NA 0.80092025	1.946371e+00	TRP	23.880425
## 1377	NA 0.98259969	4.492874e-01	TRP	23.880425
## 1378	NA 0.77523479	1.360153e+00	TRP	23.880425
## 1379	NA 0.80984149	-3.145616e-01	TRP	23.880425
## 1380	NA 0.74289258	1.819703e+00	TRP	23.880425
## 1381	NA 0.76810327	1.592278e+00	TRP	23.880425
## 1382	NA 0.70895800	3.222187e+00	TRP	23.880425

## 1383	NA 0.74006627	1.511619e-01	TRP	23.880425
## 1384	NA 0.74518337	-3.005156e-01	TRP	23.880425
## 1385	NA 0.76207541	2.343171e+00	TRP	23.880425
## 1386	NA 0.81716615	1.717553e+00	TRP	23.880425
## 1387	NA 0.82381678	1.972376e+00	TRP	23.880425
## 1388	NA 0.80568764	9.946951e-01	TRP	23.880425
## 1389	NA 0.70767673	8.085764e-01	TRP	23.880425
## 1390	NA 0.78496810	-3.928476e-01	SER	21.829007
## 1391	NA 0.84714452	-3.869216e-01	SER	21.829007
## 1392	NA 0.81731300	8.343665e-01	SER	21.829007
## 1393	NA 0.74571211	8.428612e-01	SER	21.829007
## 1394	NA 0.69771983	-5.920372e-01	SER	21.829007
## 1395	NA 0.84432168	9.784331e-02	SER	21.829007
## 1396	NA 0.78964305	-1.862352e-01	SER	21.829007
## 1397	NA 0.79762248	5.471223e-02	SER	21.829007
## 1398	NA 0.77147852	-1.008250e-01	SER	21.829007
## 1399	NA 0.79400229	-2.906159e-01	SER	21.829007
## 1400	NA 0.78452620	2.365069e-01	SER	21.829007
## 1401	NA 0.68034767	1.036774e-01	SER	21.829007
## 1402	NA 0.86355591	3.937146e-01	SER	21.829007
## 1403	NA 0.82054168	1.103129e-01	SER	21.829007
## 1404	NA 0.73793858	-5.038742e-02	SER	21.829007
## 1405	NA 0.85585510	-2.370590e-01	SER	21.829007
## 1406	NA 0.42687248	4.021300e-01	SER	21.829007
## 1407	NA 0.60798335	7.191311e-01	VAL	21.493165
## 1408	NA 0.73954432	4.143260e-01	VAL	21.493165
## 1409	NA 0.78139024	-1.931145e-01	VAL	21.493165
## 1410	NA 0.84187791	-3.877329e-01	VAL	21.493165
## 1411	NA 0.68981874	5.002514e-01	VAL	21.493165
## 1412	NA 0.69035161	2.015803e-01	VAL	21.493165
## 1413	NA 0.78149040	-1.441355e-01	VAL	21.493165
## 1414	NA 0.87319260	-1.999792e-01	VAL	21.493165
## 1415	NA 0.78098109	-3.681309e-01	VAL	21.493165
## 1416	NA 0.91136692	-2.096874e-01	VAL	21.493165
## 1417	804845 0.73973074	1.392685e-01	VAL	21.493165
## 1418	NA 0.49952660	7.640625e-01	VAL	21.493165
## 1419	NA 0.58899394	1.650293e-01	VAL	21.493165
## 1420	NA 0.73219624	8.453735e-01	VAL	21.493165
## 1421	NA 0.70696111	-1.442775e-01	VAL	21.493165
## 1422	NA 0.54232366	3.916370e-01	VAL	21.493165
## 1423	NA 0.72574386	4.469024e-02	VAL	21.493165
## 1424	NA 0.75102864	6.265434e-01	VAL	21.493165
## 1425	NA 0.61765235	1.184267e-01	VAL	21.493165
## 1426	NA 0.83929274	-6.583705e-01	LYS	20.134816
## 1427	NA 0.75739000	1.116685e+00	LYS	20.134816
## 1428	NA 0.82535443	1.290367e-01	LYS	20.134816
## 1429	NA 0.65848118	2.715447e-01	LYS	20.134816
## 1430	NA 0.83166142	-3.385045e-02	LYS	20.134816
## 1431	NA 0.73479981	-5.298896e-01	LYS	20.134816
## 1432	NA 0.72821712	1.581373e-01	LYS	20.134816
## 1433	NA 0.68296060	3.659672e-01	LYS	20.134816
## 1434	NA 0.71530337	-4.106372e-01	LYS	20.134816
## 1435	NA 0.75436841	-2.438857e-01	LYS	20.134816
## 1436	NA 0.78230095	-9.295230e-01	LYS	20.134816

## 1437	NA	0.74714761	-1.404088e-01	LYS	20.134816
## 1438	NA	0.50392364	-6.929115e-01	LYS	20.134816
## 1439	NA	0.82564652	-9.329609e-01	LYS	20.134816
## 1440	NA	0.89025699	7.323032e-01	LYS	20.134816
## 1441	NA	0.19250188	-6.617922e-02	LYS	20.134816
## 1442	NA	0.67783065	6.439361e-01	LYS	20.134816
## 1443	NA	0.81372506	-1.137308e-01	THR	23.310826
## 1444	NA	0.83965833	-3.131297e-01	THR	23.310826
## 1445	NA	0.46124799	5.824391e-01	THR	23.310826
## 1446	NA	0.74364578	6.486070e-01	THR	23.310826
## 1447	NA	0.73641591	-8.288717e-01	THR	23.310826
## 1448	NA	0.68554724	-6.634558e-02	THR	23.310826
## 1449	NA	0.82829704	2.647297e-02	THR	23.310826
## 1450	NA	0.66762383	-7.149736e-01	THR	23.310826
## 1451	NA	0.74331268	-7.875420e-01	THR	23.310826
## 1452	NA	0.74284239	-6.513792e-01	THR	23.310826
## 1453	NA	0.64731769	-3.684630e-01	THR	23.310826
## 1454	NA	0.77348147	-1.817996e-01	THR	23.310826
## 1455	NA	0.29969222	5.464301e-01	THR	23.310826
## 1456	NA	0.67451600	-4.590283e-01	THR	23.310826
## 1457	NA	0.43966081	-1.767353e-01	THR	23.310826
## 1458	2136529	0.72129866	9.399934e-01	THR	23.310826
## 1459	NA	0.74774926	-7.842267e-01	THR	23.310826
## 1460	NA	0.65652009	-2.620988e-01	THR	23.310826
## 1461	NA	0.73100928	-2.596878e-01	THR	23.310826
## 1462	NA	0.84641096	4.242226e-01	LYS	22.482805
## 1463	NA	0.81946154	5.222063e-01	LYS	22.482805
## 1464	NA	0.75669074	-3.390468e-02	LYS	22.482805
## 1465	NA	0.75162568	6.498679e-01	LYS	22.482805
## 1466	NA	0.76111584	-3.894917e-02	LYS	22.482805
## 1467	NA	0.70876598	-9.979138e-02	LYS	22.482805
## 1468	NA	0.72977227	-2.921050e-01	LYS	22.482805
## 1469	NA	0.80805202	-3.192635e-01	LYS	22.482805
## 1470	NA	0.68243467	3.148552e-01	LYS	22.482805
## 1471	NA	0.78192625	1.074440e+00	LYS	22.482805
## 1472	NA	0.73174265	-2.590925e-01	LYS	22.482805
## 1473	NA	0.69511103	4.388048e-01	LYS	22.482805
## 1474	NA	0.52414315	5.484382e-01	LYS	22.482805
## 1475	NA	0.83447769	4.898101e-01	LYS	22.482805
## 1476	NA	0.75151014	1.429385e-01	LYS	22.482805
## 1477	NA	0.70298519	-3.757239e-02	LYS	22.482805
## 1478	NA	0.82598603	3.359831e-01	LYS	22.482805
## 1479	NA	0.81048083	-6.223895e-01	LYS	22.482805
## 1480	NA	0.66362866	3.009417e-01	LYS	22.482805
## 1481	NA	0.84504284	-8.946246e-01	HIS	19.561438
## 1482	NA	0.25078442	2.954020e-02	HIS	19.561438
## 1483	NA	0.36824472	2.414696e-01	HIS	19.561438
## 1484	NA	0.92747570	-1.022917e+00	HIS	19.561438
## 1485	NA	0.85208952	-5.270572e-01	HIS	19.561438
## 1486	NA	0.82002657	1.625383e-02	HIS	19.561438
## 1487	NA	0.76055403	-6.636678e-01	HIS	19.561438
## 1488	3594719	0.60777402	2.949546e-01	HIS	19.561438
## 1489	NA	0.17449818	1.794881e-01	HIS	19.561438
## 1490	NA	0.69672019	7.015704e-01	HIS	19.561438

## 1491		NA 0.64190583	1.978591e-01	HIS	19.561438
## 1492	2093260	0.83146256	-2.393234e-01	HIS	19.561438
## 1493		NA 0.75614998	-4.052333e-01	HIS	19.561438
## 1494		NA 0.72708219	1.412856e+00	HIS	19.561438
## 1495		NA 0.79001918	-1.400620e-01	HIS	19.561438
## 1496		NA 0.78750603	9.789865e-02	HIS	19.561438
## 1497		NA 0.71183372	-5.710020e-01	HIS	19.561438
## 1498		NA 0.81191893	1.146415e-01	HIS	19.561438
## 1499		NA 0.85478285	-7.188247e-01	HIS	19.561438
## 1500		NA 0.65603796	-2.756295e-02	GLN	19.106727
## 1501		NA 0.80382226	-3.732100e-01	GLN	19.106727
## 1502		NA 0.86365313	-2.036929e-01	GLN	19.106727
## 1503		NA 0.62199035	7.974039e-02	GLN	19.106727
## 1504		NA 0.79151321	2.735632e-01	GLN	19.106727
## 1505		NA 0.82799807	-3.693043e-01	GLN	19.106727
## 1506		NA 0.82561179	1.965991e-01	GLN	19.106727
## 1507		NA 0.76511841	-3.321937e-01	GLN	19.106727
## 1508		NA 0.75062025	1.080619e-01	GLN	19.106727
## 1509		NA 0.80786031	-1.448900e-01	GLN	19.106727
## 1510		NA 0.78598118	9.515631e-02	GLN	19.106727
## 1511		NA 0.84958088	1.647026e-01	GLN	19.106727
## 1512	2576969	0.29142703	-4.162752e-01	GLN	19.106727
## 1513		NA 0.74964748	-6.440861e-01	GLN	19.106727
## 1514		NA 0.81626588	-3.894560e-01	GLN	19.106727
## 1515		NA 0.80001197	-2.338960e-02	GLN	19.106727
## 1516		NA 0.86485034	5.715953e-02	GLN	19.106727
## 1517		NA 0.67362211	1.005513e-01	GLN	19.106727
## 1518		NA 0.79504852	-8.473106e-01	MET	16.802938
## 1519		NA 0.78446265	-4.409138e-01	MET	16.802938
## 1520		NA 0.75463977	-3.943745e-01	MET	16.802938
## 1521		NA 0.81906555	-5.957683e-01	MET	16.802938
## 1522		NA 0.86647641	-4.902999e-01	MET	16.802938
## 1523		NA 0.84129901	-2.123782e-01	MET	16.802938
## 1524		NA 0.70631702	-3.230189e-01	MET	16.802938
## 1525		NA 0.86720451	-6.206217e-01	MET	16.802938
## 1526		NA 0.82911510	-4.102608e-01	MET	16.802938
## 1527		NA 0.83575332	-3.582271e-01	MET	16.802938
## 1528		NA 0.65433884	9.713561e-01	MET	16.802938
## 1529		NA 0.83023503	-3.732217e-01	MET	16.802938
## 1530		NA 0.84858078	2.053609e-01	MET	16.802938
## 1531		NA 0.85587446	6.555708e-01	MET	16.802938
## 1532		NA 0.75991728	-4.628968e-01	MET	16.802938
## 1533		NA 0.75709090	-1.580652e-01	MET	16.802938
## 1534		NA 0.83838846	-1.636836e-01	MET	16.802938
## 1535		NA 0.78905208	-3.950036e-01	MET	16.802938
## 1536		NA 0.89687544	-7.097475e-01	MET	16.802938
## 1537		NA 0.42418842	-3.678410e-01	TYR	17.418900
## 1538		NA 0.69527008	-6.510250e-01	TYR	17.418900
## 1539		NA 0.31639319	-6.309748e-01	TYR	17.418900
## 1540		NA 0.42086587	-5.210895e-01	TYR	17.418900
## 1541		NA 0.88887045	-2.762480e-01	TYR	17.418900
## 1542		NA 0.35271198	-2.208872e-01	TYR	17.418900
## 1543	585918	0.53449380	-7.771506e-01	TYR	17.418900
## 1544		NA 0.75601743	-7.817744e-01	TYR	17.418900

## 1545	NA 0.67845369	-9.562456e-01	TYR	17.418900
## 1546	NA 0.18102878	-4.528210e-01	TYR	17.418900
## 1547	NA 0.28314940	-3.501026e-01	TYR	17.418900
## 1548	NA 0.77196654	-9.020672e-01	TYR	17.418900
## 1549	NA 0.18307575	1.941787e-02	TYR	17.418900
## 1550	NA 0.38654745	-3.666818e-01	TYR	17.418900
## 1551	NA 0.33495977	-3.958044e-01	TYR	17.418900
## 1552	NA 0.34534499	-4.006015e-01	TYR	17.418900
## 1553	NA 0.24300981	-2.908419e-01	TYR	17.418900
## 1554	NA 0.57242929	-8.600114e-01	TYR	17.418900
## 1555	NA 0.83288180	-1.165177e+00	TYR	17.418900
## 1556	NA 0.81645542	-1.987956e-01	SER	16.631219
## 1557	NA 0.76032141	1.882182e-01	SER	16.631219
## 1558	NA 0.92968391	-7.855119e-01	SER	16.631219
## 1559	NA 0.90075151	-5.289523e-01	SER	16.631219
## 1560	NA 0.58664470	3.903467e-01	SER	16.631219
## 1561	NA 0.75236637	-5.854570e-01	SER	16.631219
## 1562	NA 0.76312682	-5.200267e-03	SER	16.631219
## 1563	NA 0.67046866	-3.308064e-01	SER	16.631219
## 1564	NA 0.87946482	-8.939787e-02	SER	16.631219
## 1565	NA 0.80511450	-7.959629e-01	SER	16.631219
## 1566	NA 0.83818910	-7.469166e-01	SER	16.631219
## 1567	NA 0.82163325	-2.568772e-01	SER	16.631219
## 1568	NA 0.97244280	-1.228673e+00	SER	16.631219
## 1569	NA 0.81871437	-5.356129e-01	SER	16.631219
## 1570	NA 0.86324183	-4.601301e-01	SER	16.631219
## 1571	NA 0.70419808	6.684222e-01	SER	16.631219
## 1572	NA 0.81048652	-2.568117e-01	SER	16.631219
## 1573	NA 0.73953077	-2.828616e-01	SER	16.631219
## 1574	NA 0.74619348	3.838773e-01	SER	16.631219
## 1575	NA 0.20143353	-2.392476e-01	ILE	15.742181
## 1576	NA 0.66368926	-8.513374e-01	ILE	15.742181
## 1577	NA 0.10434685	-4.265615e-01	ILE	15.742181
## 1578	NA 0.14933976	1.084544e-01	ILE	15.742181
## 1579	NA 0.61584814	-3.385679e-01	ILE	15.742181
## 1580	NA 0.84830020	2.566217e-01	ILE	15.742181
## 1581	NA 0.81637471	-2.919549e-01	ILE	15.742181
## 1582	NA 0.41000329	-4.163569e-03	ILE	15.742181
## 1583	NA 0.82020089	3.560553e-01	ILE	15.742181
## 1584	NA 0.69349975	-7.820679e-01	ILE	15.742181
## 1585	NA 0.42382605	-5.199339e-01	ILE	15.742181
## 1586	NA 0.64715184	-1.010435e+00	ILE	15.742181
## 1587	NA 0.76408724	-4.713983e-01	ILE	15.742181
## 1588	NA 0.74214669	-4.691346e-01	ILE	15.742181
## 1589	NA 0.29005097	-5.891243e-01	ILE	15.742181
## 1590	NA 0.11105835	-3.476518e-01	ILE	15.742181
## 1591	NA 0.15894548	9.944715e-02	ILE	15.742181
## 1592	NA 0.25635836	2.830644e-02	ILE	15.742181
## 1593	3339934 0.53561247	-3.342608e-01	ILE	15.742181
## 1594	NA 0.65907435	-4.284775e-01	PRO	19.142860
## 1595	NA 0.79862703	-1.615269e-02	PRO	19.142860
## 1596	NA 0.87797015	-1.018405e-01	PRO	19.142860
## 1597	NA 0.56256930	-6.864655e-01	PRO	19.142860
## 1598	NA 0.78148728	-1.157534e-01	PRO	19.142860

## 1599	NA	0.66241824	3.950633e-01	PRO	19.142860
## 1600	NA	0.76750983	3.862531e-01	PRO	19.142860
## 1601	NA	0.27685798	-1.024344e-01	PRO	19.142860
## 1602	NA	0.75339501	1.654196e-01	PRO	19.142860
## 1603	NA	0.82506672	-3.463800e-01	PRO	19.142860
## 1604	NA	0.48346676	-2.239205e-01	PRO	19.142860
## 1605	NA	0.68137727	-3.408923e-01	PRO	19.142860
## 1606	NA	0.86487202	2.517261e-02	PRO	19.142860
## 1607	NA	0.50054667	1.702145e-01	PRO	19.142860
## 1608	NA	0.76774287	-1.685099e-01	PRO	19.142860
## 1609	NA	0.38831191	-1.498618e-01	PRO	19.142860
## 1610	NA	0.85794014	2.795733e-01	PRO	19.142860
## 1611	NA	0.34843485	-1.442408e-01	PRO	19.142860
## 1612	NA	0.90245785	2.094491e-01	PRO	19.142860
## 1613	NA	0.76450047	9.466398e-01	GLU	20.165673
## 1614	NA	0.75828536	2.605208e-01	GLU	20.165673
## 1615	NA	0.80618347	2.512068e-01	GLU	20.165673
## 1616	NA	0.56673033	-5.707983e-01	GLU	20.165673
## 1617	NA	0.73836674	7.063105e-02	GLU	20.165673
## 1618	NA	0.78976368	-2.462835e-01	GLU	20.165673
## 1619	NA	0.74550534	1.389972e-01	GLU	20.165673
## 1620	NA	0.61859506	3.991004e-01	GLU	20.165673
## 1621	NA	0.78904444	7.526769e-01	GLU	20.165673
## 1622	NA	0.73605214	4.373042e-02	GLU	20.165673
## 1623	NA	0.82738148	1.909826e-01	GLU	20.165673
## 1624	NA	0.75076018	2.623013e-01	GLU	20.165673
## 1625	NA	0.72822142	2.344251e-01	GLU	20.165673
## 1626	NA	0.75232336	2.570073e-01	GLU	20.165673
## 1627	NA	0.75518896	4.564857e-01	GLU	20.165673
## 1628	NA	0.84957208	1.350523e-01	GLU	20.165673
## 1629	2882758	0.90472298	-3.331353e-01	GLU	20.165673
## 1630	NA	0.73747222	1.209476e-01	GLU	20.165673
## 1631	NA	0.74721806	3.126492e-01	GLU	20.165673
## 1632	NA	0.82936223	-2.771411e-03	ASP	21.705077
## 1633	NA	0.73078836	-7.405925e-02	ASP	21.705077
## 1634	NA	0.85393430	4.364667e-01	ASP	21.705077
## 1635	NA	0.83936167	2.196293e-01	ASP	21.705077
## 1636	NA	0.84350237	-3.773250e-01	ASP	21.705077
## 1637	NA	0.73963090	1.816002e-01	ASP	21.705077
## 1638	NA	0.84538803	2.647889e-01	ASP	21.705077
## 1639	NA	0.82999404	5.406153e-02	ASP	21.705077
## 1640	NA	0.83043368	9.586114e-02	ASP	21.705077
## 1641	NA	0.76279901	2.913094e-01	ASP	21.705077
## 1642	NA	0.78231851	9.158746e-01	ASP	21.705077
## 1643	NA	0.82342604	2.929366e-01	ASP	21.705077
## 1644	NA	0.83395889	4.856137e-01	ASP	21.705077
## 1645	NA	0.82713669	3.821513e-01	ASP	21.705077
## 1646	NA	0.82476676	3.103312e-01	ASP	21.705077
## 1647	NA	0.85178617	-2.105160e-01	ASP	21.705077
## 1648	NA	0.87107897	1.981396e-01	ASP	21.705077
## 1649	NA	0.88468398	5.619144e-02	ASP	21.705077
## 1650	NA	0.83292672	-1.012592e-01	ASP	21.705077
## 1651	NA	0.83573804	1.016712e+00	ALA	18.925511
## 1652	NA	0.83713848	-1.364022e-01	ALA	18.925511

## 1653	NA	0.85870847	-7.367866e-02	ALA	18.925511
## 1654	NA	0.77292224	3.558201e-01	ALA	18.925511
## 1655	NA	0.86690036	-7.248987e-01	ALA	18.925511
## 1656	NA	0.82180428	7.509808e-01	ALA	18.925511
## 1657	NA	0.72962243	4.733575e-01	ALA	18.925511
## 1658	NA	0.65106598	-4.686740e-01	ALA	18.925511
## 1659	NA	0.88668462	6.330903e-01	ALA	18.925511
## 1660	NA	0.98726515	9.134530e-02	ALA	18.925511
## 1661	NA	0.86326770	2.385847e-01	ALA	18.925511
## 1662	NA	0.82603168	-3.757206e-02	ALA	18.925511
## 1663	NA	0.76048723	-5.426823e-01	ALA	18.925511
## 1664	NA	0.77241187	2.942361e-01	ALA	18.925511
## 1665	NA	0.73641211	1.558537e-01	ALA	18.925511
## 1666	NA	0.61017731	4.862219e-03	ALA	18.925511
## 1667	NA	0.72831019	4.232323e-01	ALA	18.925511
## 1668	NA	0.80468590	-3.296276e-01	ALA	18.925511
## 1669	NA	0.53591829	-6.223640e-01	MET	16.402310
## 1670	NA	0.85120057	-2.642083e-01	MET	16.402310
## 1671	NA	0.83252392	-3.281373e-01	MET	16.402310
## 1672	NA	0.74595906	-9.873440e-01	MET	16.402310
## 1673	NA	0.84056036	-6.727135e-01	MET	16.402310
## 1674	NA	0.86543431	5.538393e-01	MET	16.402310
## 1675	NA	0.85633294	6.677960e-02	MET	16.402310
## 1676	NA	0.75657251	9.595650e-01	MET	16.402310
## 1677	NA	0.81400130	-4.648360e-01	MET	16.402310
## 1678	NA	0.81955694	-8.809031e-01	MET	16.402310
## 1679	NA	0.83966440	-5.534969e-01	MET	16.402310
## 1680	NA	0.74131461	-7.374449e-01	MET	16.402310
## 1681	NA	0.79447420	-9.026991e-01	MET	16.402310
## 1682	NA	0.59002194	-1.348769e-01	MET	16.402310
## 1683	NA	0.79956004	-5.471528e-01	MET	16.402310
## 1684	NA	0.71673115	5.546581e-01	MET	16.402310
## 1685	2684205	0.75376473	-2.394346e-01	MET	16.402310
## 1686	NA	0.75930235	-5.398635e-01	MET	16.402310
## 1687	NA	0.87548327	-3.255167e-01	THR	18.597542
## 1688	NA	0.84943056	8.675191e-02	THR	18.597542
## 1689	NA	0.88801895	-5.676833e-01	THR	18.597542
## 1690	NA	0.84796691	-9.473910e-01	THR	18.597542
## 1691	NA	0.84032629	-3.477820e-01	THR	18.597542
## 1692	NA	0.68440660	5.470655e-02	THR	18.597542
## 1693	NA	0.54677385	1.663613e-01	THR	18.597542
## 1694	NA	0.84261328	-3.752495e-01	THR	18.597542
## 1695	NA	0.73009518	-1.584268e-01	THR	18.597542
## 1696	NA	0.82301972	2.321731e-01	THR	18.597542
## 1697	NA	0.66419751	2.826028e-02	THR	18.597542
## 1698	NA	0.45553342	-6.892273e-01	THR	18.597542
## 1699	NA	0.91489610	-6.824329e-01	THR	18.597542
## 1700	NA	0.83915278	-4.941537e-01	THR	18.597542
## 1701	NA	0.75436730	-7.860849e-02	THR	18.597542
## 1702	NA	0.74281906	4.154538e-01	THR	18.597542
## 1703	NA	0.66671299	-5.986513e-01	THR	18.597542
## 1704	NA	0.79151775	-8.596594e-01	THR	18.597542
## 1705	NA	0.75946350	-1.128857e+00	GLY	20.142450
## 1706	NA	0.24292222	-3.992874e-01	GLY	20.142450

## 1707	NA	0.60271882	6.645229e-01	GLY	20.142450
## 1708	NA	0.71530993	-5.769462e-01	GLY	20.142450
## 1709	NA	0.77607762	-7.380895e-01	GLY	20.142450
## 1710	NA	0.81057394	-6.914639e-01	GLY	20.142450
## 1711	NA	0.45543137	-1.604797e-01	GLY	20.142450
## 1712	NA	0.69726586	5.626258e-01	GLY	20.142450
## 1713	NA	0.24118682	3.919830e-01	GLY	20.142450
## 1714	NA	0.77029444	-2.020512e-01	GLY	20.142450
## 1715	NA	0.43839705	-1.873284e-01	GLY	20.142450
## 1716	NA	0.84181419	-4.701071e-01	GLY	20.142450
## 1717	1496579	0.54276900	-1.907035e-01	GLY	20.142450
## 1718	NA	0.75068416	-7.254142e-01	GLY	20.142450
## 1719	NA	0.69622441	-3.281604e-01	GLY	20.142450
## 1720	NA	0.46089966	3.531348e-01	GLY	20.142450
## 1721	NA	0.82354988	1.776498e-01	GLY	20.142450
## 1722	NA	0.68990382	-6.125463e-01	GLY	20.142450
## 1723	NA	0.79638357	-7.279159e-01	GLY	20.142450
## 1724	NA	0.73851238	-8.323884e-01	THR	19.192291
## 1725	NA	0.79064694	-3.873164e-01	THR	19.192291
## 1726	NA	0.68556282	-4.903322e-01	THR	19.192291
## 1727	NA	0.81420831	-8.673920e-01	THR	19.192291
## 1728	NA	0.65108718	-9.020218e-01	THR	19.192291
## 1729	NA	0.73874095	-6.476283e-01	THR	19.192291
## 1730	NA	0.64047161	-4.420111e-01	THR	19.192291
## 1731	NA	0.47034410	-4.246713e-01	THR	19.192291
## 1732	NA	0.38345874	-3.856957e-01	THR	19.192291
## 1733	NA	0.85297364	-9.277196e-01	THR	19.192291
## 1734	NA	0.78202595	-9.102674e-01	THR	19.192291
## 1735	NA	0.71091442	-1.230446e+00	THR	19.192291
## 1736	NA	0.90608318	-3.457535e-01	THR	19.192291
## 1737	NA	0.82742160	-6.678241e-01	THR	19.192291
## 1738	NA	0.74665548	1.402470e-01	THR	19.192291
## 1739	NA	0.71730972	-6.354195e-01	THR	19.192291
## 1740	NA	0.65574195	-7.734523e-01	THR	19.192291
## 1741	NA	0.57711254	-6.580786e-01	THR	19.192291
## 1742	NA	0.70302938	-8.309411e-01	ALA	16.928415
## 1743	NA	0.75083009	-1.124713e+00	ALA	16.928415
## 1744	NA	0.80202361	-9.749447e-01	ALA	16.928415
## 1745	NA	0.66277499	-5.619161e-01	ALA	16.928415
## 1746	NA	0.78671523	-1.061315e+00	ALA	16.928415
## 1747	NA	0.78026404	-9.732349e-01	ALA	16.928415
## 1748	NA	0.79362153	-9.273316e-01	ALA	16.928415
## 1749	NA	0.74445543	-6.278901e-01	ALA	16.928415
## 1750	NA	0.72631537	-8.756939e-01	ALA	16.928415
## 1751	NA	0.77311790	-8.783535e-01	ALA	16.928415
## 1752	NA	0.86554341	6.392435e-01	ALA	16.928415
## 1753	NA	0.72302633	-1.049952e+00	ALA	16.928415
## 1754	1338287	0.74044023	-8.570981e-01	ALA	16.928415
## 1755	NA	0.80508366	3.876503e-01	ALA	16.928415
## 1756	NA	0.81142451	-5.727936e-01	ALA	16.928415
## 1757	NA	0.75851839	-3.547875e-01	ALA	16.928415
## 1758	NA	0.83679953	-1.025811e+00	ALA	16.928415
## 1759	NA	0.67423881	-8.495981e-01	ALA	16.928415
## 1760	NA	0.82403800	-7.154898e-01	ALA	16.928415

## 1761	NA	0.65316226	-1.678461e-01	GLU	20.327096
## 1762	NA	0.61910165	7.041347e-01	GLU	20.327096
## 1763	NA	0.72187192	-2.529304e-01	GLU	20.327096
## 1764	NA	0.79619280	5.139759e-01	GLU	20.327096
## 1765	NA	0.63436863	-1.000646e+00	GLU	20.327096
## 1766	NA	0.72183971	-8.431697e-01	GLU	20.327096
## 1767	NA	0.61692162	-2.125548e-01	GLU	20.327096
## 1768	NA	0.87661895	-1.635952e-01	GLU	20.327096
## 1769	NA	0.55155344	2.803350e-01	GLU	20.327096
## 1770	NA	0.86933112	-3.350969e-01	GLU	20.327096
## 1771	NA	0.59898517	1.518738e-01	GLU	20.327096
## 1772	NA	0.08629798	6.625701e-01	GLU	20.327096
## 1773	NA	0.76325207	-1.402411e-01	GLU	20.327096
## 1774	NA	0.30698324	4.652159e-01	GLU	20.327096
## 1775	NA	0.63418665	3.916176e-01	GLU	20.327096
## 1776	NA	0.25512103	1.002959e+00	GLU	20.327096
## 1777	NA	0.81173695	9.843786e-02	GLU	20.327096
## 1778	NA	0.71003313	-6.263503e-01	GLU	20.327096
## 1779	NA	0.73379128	-2.786844e-01	GLU	20.327096
## 1780	NA	0.68298731	-3.274174e-01	MET	21.045411
## 1781	NA	0.86885584	-1.239426e-02	MET	21.045411
## 1782	NA	0.74805325	-3.106183e-01	MET	21.045411
## 1783	NA	0.86939608	-3.159747e-01	MET	21.045411
## 1784	NA	0.84536819	-2.566334e-01	MET	21.045411
## 1785	NA	0.76021080	-3.615943e-02	MET	21.045411
## 1786	NA	0.84160864	-8.559330e-02	MET	21.045411
## 1787	NA	0.78953637	3.854042e-02	MET	21.045411
## 1788	NA	0.84234206	7.582914e-01	MET	21.045411
## 1789	NA	0.77565912	-1.106962e-01	MET	21.045411
## 1790	NA	0.57391646	-5.680061e-01	MET	21.045411
## 1791	NA	0.84898195	3.524815e-01	MET	21.045411
## 1792	NA	0.78206630	-5.119299e-01	MET	21.045411
## 1793	NA	0.83436749	-6.486974e-01	MET	21.045411
## 1794	NA	0.73680188	-2.947118e-01	MET	21.045411
## 1795	NA	0.58382626	-1.198119e-01	MET	21.045411
## 1796	NA	0.66837908	-4.188548e-01	MET	21.045411
## 1797	NA	0.74677476	-5.183932e-01	MET	21.045411
## 1798	NA	0.74091904	-1.206981e-01	MET	21.045411
## 1799	NA	0.60583315	-1.091921e-01	LEU	17.601613
## 1800	NA	0.67749607	-8.067842e-01	LEU	17.601613
## 1801	NA	0.65524309	-5.307201e-01	LEU	17.601613
## 1802	NA	0.54724808	-5.007362e-01	LEU	17.601613
## 1803	NA	0.76000921	-8.262283e-01	LEU	17.601613
## 1804	NA	0.60749360	-9.023130e-01	LEU	17.601613
## 1805	NA	0.67987476	-8.859797e-01	LEU	17.601613
## 1806	NA	0.76483827	-8.595761e-01	LEU	17.601613
## 1807	NA	0.79378656	-9.680076e-01	LEU	17.601613
## 1808	435307	0.74924281	-3.002182e-01	LEU	17.601613
## 1809	NA	0.70817910	-1.077103e+00	LEU	17.601613
## 1810	3338654	0.80968024	-1.149415e+00	LEU	17.601613
## 1811	NA	0.72044244	-9.596044e-01	LEU	17.601613
## 1812	NA	0.96525836	-5.673541e-01	LEU	17.601613
## 1813	NA	0.87628373	-9.946251e-01	LEU	17.601613
## 1814	NA	0.66652514	-9.412020e-01	LEU	17.601613

## 1815	NA 0.49933106	-4.531604e-01	LEU	17.601613
## 1816	NA 0.86531285	-9.813140e-01	LEU	17.601613
## 1817	NA 0.62412680	-2.912155e-01	PHE	17.962187
## 1818	NA 0.62565331	-1.250052e+00	PHE	17.962187
## 1819	NA 0.69146402	-6.773423e-01	PHE	17.962187
## 1820	NA 0.32033902	-3.342865e-01	PHE	17.962187
## 1821	NA 0.73603317	-7.476009e-01	PHE	17.962187
## 1822	NA 0.39040379	-5.169248e-01	PHE	17.962187
## 1823	NA 0.78653021	-8.041837e-01	PHE	17.962187
## 1824	NA 0.82352918	-1.261819e+00	PHE	17.962187
## 1825	NA 0.17045879	-4.841152e-01	PHE	17.962187
## 1826	NA 0.66046051	-9.446040e-01	PHE	17.962187
## 1827	NA 0.87781031	-8.105290e-01	PHE	17.962187
## 1828	NA 0.30585813	-3.507704e-01	PHE	17.962187
## 1829	NA 0.48182345	-4.050352e-01	PHE	17.962187
## 1830	NA 0.43969410	-5.975540e-01	PHE	17.962187
## 1831	NA 0.32430261	-6.776301e-01	PHE	17.962187
## 1832	NA 0.75775764	-1.246147e+00	PHE	17.962187
## 1833	NA 0.76026242	-8.842029e-01	PHE	17.962187
## 1834	NA 0.23528619	-5.242453e-01	PHE	17.962187
## 1835	NA 0.78284447	-8.524974e-01	PHE	17.962187
## 1836	NA 0.70889233	-5.362135e-01	ASP	21.678584
## 1837	NA 0.19921921	-4.905770e-01	ASP	21.678584
## 1838	NA 0.28386538	-4.817603e-01	ASP	21.678584
## 1839	NA 0.64326215	-2.975234e-01	ASP	21.678584
## 1840	NA 0.63841576	-4.877241e-01	ASP	21.678584
## 1841	NA 0.63841187	-3.820398e-01	ASP	21.678584
## 1842	NA 0.40782078	-6.401618e-01	ASP	21.678584
## 1843	NA 0.53780110	-9.203883e-02	ASP	21.678584
## 1844	NA 0.30365066	-8.152593e-02	ASP	21.678584
## 1845	NA 0.68745924	-5.648772e-01	ASP	21.678584
## 1846	NA 0.29367931	-1.853212e-01	ASP	21.678584
## 1847	NA 0.57292830	-6.237080e-01	ASP	21.678584
## 1848	NA 0.66354977	-4.391688e-01	ASP	21.678584
## 1849	NA 0.49197840	-4.437794e-01	ASP	21.678584
## 1850	NA 0.46476231	-6.342473e-01	ASP	21.678584
## 1851	NA 0.72711871	-7.352078e-01	ASP	21.678584
## 1852	NA 0.68554388	-6.656343e-01	TYR	20.759327
## 1853	NA 0.67712324	-5.664230e-01	TYR	20.759327
## 1854	NA 0.34237370	-3.107181e-01	TYR	20.759327
## 1855	NA 0.77844476	-9.679117e-01	TYR	20.759327
## 1856	NA 0.88665348	-5.279973e-01	TYR	20.759327
## 1857	NA 0.37043180	7.649880e-01	TYR	20.759327
## 1858	NA 0.73787695	1.132150e-01	TYR	20.759327
## 1859	NA 0.75446946	-4.823965e-01	TYR	20.759327
## 1860	NA 0.22192235	1.889781e-01	TYR	20.759327
## 1861	NA 0.71258952	-5.899309e-01	TYR	20.759327
## 1862	NA 0.59583924	-8.409601e-01	TYR	20.759327
## 1863	NA 0.58815921	-6.073861e-01	TYR	20.759327
## 1864	NA 0.40272872	-4.344490e-01	TYR	20.759327
## 1865	NA 0.84440623	-8.353588e-01	TYR	20.759327
## 1866	NA 0.59804482	-4.044394e-01	TYR	20.759327
## 1867	NA 0.76097229	-6.128337e-01	TYR	20.759327
## 1868	NA 0.33272774	-3.398754e-01	TYR	20.759327

## 1869	NA 0.77262550	-6.599122e-01	TYR	20.759327
## 1870	NA 0.73469951	-9.611854e-01	TYR	20.759327
## 1871	NA 0.30652095	-6.003656e-01	ILE	18.385511
## 1872	NA 0.23763140	-4.504431e-01	ILE	18.385511
## 1873	NA 0.74026853	-9.769480e-01	ILE	18.385511
## 1874	NA 0.63578550	-5.529245e-01	ILE	18.385511
## 1875	NA 0.22364008	-1.713790e-01	ILE	18.385511
## 1876	NA 0.46438170	-3.989317e-01	ILE	18.385511
## 1877	NA 0.10939497	7.406354e-03	ILE	18.385511
## 1878	NA 0.16780117	-4.675959e-01	ILE	18.385511
## 1879	NA 0.75669209	-4.474322e-01	ILE	18.385511
## 1880	NA 0.88383288	-4.930904e-01	ILE	18.385511
## 1881	NA 0.70905345	2.910792e-01	ILE	18.385511
## 1882	NA 0.38485096	-2.056335e-01	ILE	18.385511
## 1883	NA 0.35320787	-6.731128e-01	ILE	18.385511
## 1884	NA 0.25885242	-6.499913e-01	ILE	18.385511
## 1885	NA 0.08998233	-2.866997e-01	ILE	18.385511
## 1886	NA 0.61584839	-4.236999e-01	ILE	18.385511
## 1887	NA 0.28565114	-7.921310e-01	ILE	18.385511
## 1888	NA 0.10527658	-3.205107e-01	ILE	18.385511
## 1889	NA 0.14400153	1.106740e-01	ILE	18.385511
## 1890	NA 0.77228545	3.512361e-02	SER	21.558350
## 1891	NA 0.84763366	-1.654297e-01	SER	21.558350
## 1892	NA 0.15126311	-3.498040e-01	SER	21.558350
## 1893	NA 0.72843360	-6.220318e-01	SER	21.558350
## 1894	NA 0.72476844	-1.730961e-01	SER	21.558350
## 1895	NA 0.76275670	1.091189e+00	SER	21.558350
## 1896	NA 0.38997805	-3.960478e-01	SER	21.558350
## 1897	NA 0.31892112	1.653299e-01	SER	21.558350
## 1898	NA 0.89141210	-5.568334e-01	SER	21.558350
## 1899	NA 0.59846931	-6.924167e-01	SER	21.558350
## 1900	NA 0.67845178	-1.148631e+00	SER	21.558350
## 1901	NA 0.19634300	-8.691919e-02	SER	21.558350
## 1902	NA 0.54769733	-4.630760e-01	SER	21.558350
## 1903	NA 0.72847430	-8.439026e-01	SER	21.558350
## 1904	NA 0.76469328	8.334662e-01	SER	21.558350
## 1905	NA 0.73180016	-6.184419e-01	SER	21.558350
## 1906	NA 0.86095852	9.766417e-01	GLU	23.246104
## 1907	NA 0.70716016	7.234714e-01	GLU	23.246104
## 1908	NA 0.74992155	-1.211846e-01	GLU	23.246104
## 1909	NA 0.83667692	2.338052e-01	GLU	23.246104
## 1910	NA 0.74529291	-3.318798e-01	GLU	23.246104
## 1911	NA 0.44450513	4.158500e-01	GLU	23.246104
## 1912	NA 0.59660378	-9.234929e-02	GLU	23.246104
## 1913	NA 0.78736376	3.005381e-01	GLU	23.246104
## 1914	NA 0.61986385	5.928643e-02	GLU	23.246104
## 1915	NA 0.31975973	4.148651e-01	GLU	23.246104
## 1916	NA 0.89040300	-4.204873e-01	GLU	23.246104
## 1917	NA 0.77287250	-1.678342e-01	GLU	23.246104
## 1918	NA 0.70891894	9.709282e-01	GLU	23.246104
## 1919	NA 0.69977406	4.549448e-01	GLU	23.246104
## 1920	NA 0.73159356	-2.564321e-01	GLU	23.246104
## 1921	NA 0.36291988	-4.268967e-01	GLU	23.246104
## 1922	NA 0.87552053	-5.186334e-01	GLU	23.246104

## 1923	NA	0.80631231	-9.225921e-01	GLU	23.246104
## 1924	NA	0.70040676	-5.989973e-01	CYS	20.774529
## 1925	NA	0.82524219	8.810325e-03	CYS	20.774529
## 1926	NA	0.68301219	-1.004134e+00	CYS	20.774529
## 1927	NA	0.79401215	-1.953982e-01	CYS	20.774529
## 1928	NA	0.38638746	-5.215242e-01	CYS	20.774529
## 1929	NA	0.64860262	-6.392565e-01	CYS	20.774529
## 1930	NA	0.79551672	-6.530516e-01	CYS	20.774529
## 1931	NA	0.46052795	-5.213006e-01	CYS	20.774529
## 1932	NA	0.56091979	-7.052408e-01	CYS	20.774529
## 1933	NA	0.56400495	-9.969542e-02	CYS	20.774529
## 1934	NA	0.62372635	-9.004405e-01	CYS	20.774529
## 1935	NA	0.67793102	-5.730487e-01	CYS	20.774529
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## 1937	NA	0.81369173	-1.436188e+00	CYS	20.774529
## 1938	NA	0.58853344	-2.644166e-01	CYS	20.774529
## 1939	NA	0.55007186	-3.836510e-01	CYS	20.774529
## 1940	NA	0.73788493	2.294838e-02	CYS	20.774529
## 1941	NA	0.24904002	-3.123328e-01	ILE	21.064761
## 1942	NA	0.52675350	-1.276209e-01	ILE	21.064761
## 1943	1704126	0.52830654	-9.129511e-01	ILE	21.064761
## 1944	NA	0.20174679	-4.259429e-02	ILE	21.064761
## 1945	NA	0.72285996	-9.509570e-01	ILE	21.064761
## 1946	NA	0.19099148	-4.200335e-01	ILE	21.064761
## 1947	NA	0.29372782	-4.061533e-01	ILE	21.064761
## 1948	NA	0.12294875	-3.371018e-01	ILE	21.064761
## 1949	NA	0.76787852	-4.792335e-01	ILE	21.064761
## 1950	NA	0.55680073	-3.057235e-01	ILE	21.064761
## 1951	NA	0.13999759	-5.210046e-01	ILE	21.064761
## 1952	NA	0.41890151	-8.650860e-01	ILE	21.064761
## 1953	NA	0.76375668	-3.341172e-01	ILE	21.064761
## 1954	NA	0.41426867	-6.818524e-01	ILE	21.064761
## 1955	NA	0.09569822	-2.755400e-01	ILE	21.064761
## 1956	NA	0.67173978	-5.693607e-01	ILE	21.064761
## 1957	NA	0.14855763	-2.971631e-01	ILE	21.064761
## 1958	NA	0.80664315	-8.298936e-01	SER	24.789253
## 1959	NA	0.82780273	-1.450707e-01	SER	24.789253
## 1960	NA	0.80280645	-4.761854e-01	SER	24.789253
## 1961	NA	0.96844202	-6.989985e-01	SER	24.789253
## 1962	NA	0.69565766	-3.434639e-01	SER	24.789253
## 1963	NA	0.83713488	1.074578e+00	SER	24.789253
## 1964	NA	0.75633471	-9.153306e-01	SER	24.789253
## 1965	NA	0.64467550	-2.344154e-01	SER	24.789253
## 1966	NA	0.79799403	-7.103629e-01	SER	24.789253
## 1967	NA	0.77964770	-7.330659e-01	SER	24.789253
## 1968	NA	0.42210658	3.732063e-01	SER	24.789253
## 1969	NA	0.85813869	-6.578419e-01	SER	24.789253
## 1970	16138	0.28551775	-4.587742e-01	SER	24.789253
## 1971	NA	0.45925201	-5.825149e-01	SER	24.789253
## 1972	NA	0.83207944	1.603739e-02	SER	24.789253
## 1973	NA	0.66508761	-6.827700e-01	SER	24.789253
## 1974	NA	0.86981855	-8.720764e-01	SER	24.789253
## 1975	NA	0.69084499	-4.413663e-01	SER	24.789253
## 1976	NA	0.74461366	-3.554073e-01	SER	24.789253

## 1977	NA	0.63444827	-1.079814e-01	ASP	25.048614
## 1978	NA	0.61860611	-4.696085e-01	ASP	25.048614
## 1979	NA	0.76966873	-7.494419e-01	ASP	25.048614
## 1980	NA	0.87353969	-8.194068e-02	ASP	25.048614
## 1981	NA	0.85142089	-7.720917e-01	ASP	25.048614
## 1982	NA	0.75134073	-7.455326e-01	ASP	25.048614
## 1983	NA	0.65220837	-1.060866e-01	ASP	25.048614
## 1984	NA	0.15172303	-3.873106e-01	ASP	25.048614
## 1985	NA	0.82484577	-7.444841e-01	ASP	25.048614
## 1986	NA	0.68858456	3.819044e-01	ASP	25.048614
## 1987	NA	0.73220954	-7.035998e-01	ASP	25.048614
## 1988	NA	0.70550416	-6.886573e-01	ASP	25.048614
## 1989	NA	0.79138389	-9.158717e-02	ASP	25.048614
## 1990	NA	0.49574326	2.638153e-01	ASP	25.048614
## 1991	NA	0.61166098	-7.081355e-01	ASP	25.048614
## 1992	972807	0.71914836	-1.137828e-03	ASP	25.048614
## 1993	NA	0.72076651	-1.127715e-01	ASP	25.048614
## 1994	NA	0.79956349	-1.119270e-01	ASP	25.048614
## 1995	NA	0.82248741	3.654920e-01	ASP	25.048614
## 1996	NA	0.19076944	-1.871354e-02	PHE	23.355446
## 1997	NA	0.40745926	-6.400030e-01	PHE	23.355446
## 1998	NA	0.45017922	-5.852211e-01	PHE	23.355446
## 1999	NA	0.17087633	-6.900685e-01	PHE	23.355446
## 2000	NA	0.40502204	-6.402484e-01	PHE	23.355446
## 2001	NA	0.45966134	-6.278506e-01	PHE	23.355446
## 2002	NA	0.30046829	-3.227784e-01	PHE	23.355446
## 2003	NA	0.79049520	-2.635547e-01	PHE	23.355446
## 2004	NA	0.29769363	-2.960078e-01	PHE	23.355446
## 2005	NA	0.49270013	-2.870221e-01	PHE	23.355446
## 2006	NA	0.18748503	-2.230160e-01	PHE	23.355446
## 2007	NA	0.33080206	-4.940198e-01	PHE	23.355446
## 2008	NA	0.46115079	-9.991114e-01	PHE	23.355446
## 2009	NA	0.60730459	-4.140491e-01	PHE	23.355446
## 2010	NA	0.37958638	-6.363476e-01	PHE	23.355446
## 2011	NA	0.70622478	-4.532204e-01	PHE	23.355446
## 2012	NA	0.62389010	-4.760582e-01	PHE	23.355446
## 2013	NA	0.45925054	-5.739511e-01	PHE	23.355446
## 2014	NA	0.35007904	5.835340e-02	PHE	23.355446
## 2015	NA	0.80783759	-4.212655e-01	LEU	25.948087
## 2016	NA	0.71244095	-9.536687e-01	LEU	25.948087
## 2017	NA	0.32593585	-4.545127e-01	LEU	25.948087
## 2018	NA	0.43777586	-3.939365e-01	LEU	25.948087
## 2019	NA	0.55886296	-6.466247e-01	LEU	25.948087
## 2020	NA	0.80520588	-6.255118e-01	LEU	25.948087
## 2021	NA	0.56056941	-8.132207e-01	LEU	25.948087
## 2022	NA	0.69276195	-1.098724e+00	LEU	25.948087
## 2023	NA	0.60889648	-7.036293e-01	LEU	25.948087
## 2024	NA	0.78639688	2.851644e-02	LEU	25.948087
## 2025	NA	0.45532272	-5.485820e-01	LEU	25.948087
## 2026	NA	0.50133004	-7.139149e-01	LEU	25.948087
## 2027	NA	0.76399002	-2.701480e-01	LEU	25.948087
## 2028	NA	0.15725883	-3.436291e-01	LEU	25.948087
## 2029	NA	0.59644874	-6.300206e-01	LEU	25.948087
## 2030	NA	0.49218918	-2.464197e-01	LEU	25.948087

## 2031	NA 0.22904998	-2.079273e-01	LEU	25.948087
## 2032	NA 0.49981868	2.442220e-01	ASP	28.875084
## 2033	NA 0.83020562	-5.367161e-02	ASP	28.875084
## 2034	NA 0.79036424	-7.963385e-01	ASP	28.875084
## 2035	NA 0.64577861	4.563890e-01	ASP	28.875084
## 2036	NA 0.80425026	-3.237736e-01	ASP	28.875084
## 2037	NA 0.74528105	-1.131273e-01	ASP	28.875084
## 2038	NA 0.79873428	-5.342348e-01	ASP	28.875084
## 2039	NA 0.60292996	-4.010350e-01	ASP	28.875084
## 2040	NA 0.79637161	-1.304132e-01	ASP	28.875084
## 2041	NA 0.79610846	-5.768653e-01	ASP	28.875084
## 2042	NA 0.64400946	1.100701e-01	ASP	28.875084
## 2043	NA 0.81020866	-2.527187e-01	ASP	28.875084
## 2044	NA 0.95975851	-1.924115e-01	ASP	28.875084
## 2045	NA 0.78252462	3.909283e-01	ASP	28.875084
## 2046	NA 0.82850812	5.137410e-02	ASP	28.875084
## 2047	NA 0.19458209	-8.694788e-02	ASP	28.875084
## 2048	NA 0.86301434	1.701586e-02	ASP	28.875084
## 2049	NA 0.79675481	-2.836592e-01	LYS	28.161764
## 2050	NA 0.62534566	5.621679e-01	LYS	28.161764
## 2051	NA 0.69547642	-7.909343e-01	LYS	28.161764
## 2052	NA 0.76114680	-4.775534e-01	LYS	28.161764
## 2053	NA 0.73619013	-5.569134e-02	LYS	28.161764
## 2054	NA 0.69386692	2.047592e-01	LYS	28.161764
## 2055	NA 0.74831447	-1.681607e-01	LYS	28.161764
## 2056	NA 0.79730140	-2.473552e-01	LYS	28.161764
## 2057	NA 0.56677622	-2.328303e-01	LYS	28.161764
## 2058	NA 0.70578486	-3.565730e-01	LYS	28.161764
## 2059	NA 0.70560379	5.001759e-01	LYS	28.161764
## 2060	NA 0.82168255	6.721550e-03	LYS	28.161764
## 2061	NA 0.81884929	6.657434e-01	LYS	28.161764
## 2062	NA 0.78941458	-3.173396e-01	LYS	28.161764
## 2063	NA 0.68297486	2.896306e-01	LYS	28.161764
## 2064	NA 0.76477310	1.293837e-01	LYS	28.161764
## 2065	NA 0.63999234	3.485201e-01	LYS	28.161764
## 2066	NA 0.18497265	-1.592963e-01	LYS	28.161764
## 2067	NA 0.68013850	-2.798049e-02	HIS	28.105252
## 2068	NA 0.26412475	2.901216e-01	HIS	28.105252
## 2069	NA 0.78323366	5.313514e-01	HIS	28.105252
## 2070	NA 0.60192981	5.140238e-01	HIS	28.105252
## 2071	NA 0.73644943	7.462042e-02	HIS	28.105252
## 2072	NA 0.56515072	3.727127e-01	HIS	28.105252
## 2073	NA 0.57820108	1.501643e+00	HIS	28.105252
## 2074	NA 0.73219675	5.423511e-02	HIS	28.105252
## 2075	NA 0.76329121	2.788122e-01	HIS	28.105252
## 2076	NA 0.11752589	1.771825e-01	HIS	28.105252
## 2077	NA 0.76176305	-1.868346e-01	HIS	28.105252
## 2078	NA 0.75957953	6.225105e-01	HIS	28.105252
## 2079	NA 0.49030609	-5.029033e-01	HIS	28.105252
## 2080	NA 0.78820848	1.297805e+00	HIS	28.105252
## 2081	NA 0.72819904	-1.866465e-01	HIS	28.105252
## 2082	NA 0.78920864	6.412325e-01	HIS	28.105252
## 2083	NA 0.82261189	-3.226610e-01	HIS	28.105252
## 2084	NA 0.83459595	-3.038001e-01	HIS	28.105252

## 2085	NA	0.76121305	6.533469e-01	HIS	28.105252
## 2086	NA	0.70183409	2.103393e-01	GLN	31.139989
## 2087	NA	0.69434654	1.242212e-01	GLN	31.139989
## 2088	NA	0.68882253	-6.221601e-01	GLN	31.139989
## 2089	NA	0.81882735	2.035985e-02	GLN	31.139989
## 2090	NA	0.70202435	1.095133e-02	GLN	31.139989
## 2091	NA	0.80249149	8.115873e-01	GLN	31.139989
## 2092	NA	0.72213278	-7.998445e-01	GLN	31.139989
## 2093	NA	0.45455798	2.035439e-01	GLN	31.139989
## 2094	NA	0.60014697	2.681640e-01	GLN	31.139989
## 2095	NA	0.74811379	-7.931165e-01	GLN	31.139989
## 2096	NA	0.60669080	1.896713e-01	GLN	31.139989
## 2097	NA	0.66024466	4.701834e-01	GLN	31.139989
## 2098	NA	0.47826329	-7.255760e-02	GLN	31.139989
## 2099	NA	0.63993469	-4.158733e-01	GLN	31.139989
## 2100	NA	0.78970158	3.071213e-01	GLN	31.139989
## 2101	NA	0.84625899	5.090312e-01	GLN	31.139989
## 2102	NA	0.69237650	4.094070e-01	GLN	31.139989
## 2103	NA	0.80941139	-3.775174e-01	GLN	31.139989
## 2104	NA	0.78530889	-7.633388e-01	MET	29.437060
## 2105	NA	0.76610222	-6.393687e-01	MET	29.437060
## 2106	NA	0.54829713	4.772164e-01	MET	29.437060
## 2107	NA	0.70492718	-3.835149e-01	MET	29.437060
## 2108	NA	0.75304364	-1.349791e-01	MET	29.437060
## 2109	NA	0.63507609	-4.105493e-01	MET	29.437060
## 2110	NA	0.86880493	-3.665409e-01	MET	29.437060
## 2111	NA	0.58809030	-2.573269e-01	MET	29.437060
## 2112	NA	0.76521099	6.680209e-01	MET	29.437060
## 2113	NA	0.73283007	2.069173e-02	MET	29.437060
## 2114	NA	0.81511682	-5.320457e-01	MET	29.437060
## 2115	1028584	0.87852356	-3.835083e-01	MET	29.437060
## 2116	NA	0.72066551	-7.769731e-01	MET	29.437060
## 2117	NA	0.62347846	-2.664518e-01	MET	29.437060
## 2118	NA	0.63712084	-1.797749e-01	MET	29.437060
## 2119	NA	0.67166108	-4.167531e-01	MET	29.437060
## 2120	NA	0.77726061	3.712141e-01	MET	29.437060
## 2121	NA	0.76191666	5.766403e-02	MET	29.437060
## 2122	NA	0.75774662	-5.636905e-01	LYS	29.188956
## 2123	NA	0.65781435	-8.222542e-01	LYS	29.188956
## 2124	NA	0.79990904	-4.243476e-01	LYS	29.188956
## 2125	NA	0.65149893	-4.116987e-01	LYS	29.188956
## 2126	NA	0.83588216	-7.218050e-01	LYS	29.188956
## 2127	NA	0.83166627	-5.931939e-01	LYS	29.188956
## 2128	NA	0.72479068	-6.465046e-01	LYS	29.188956
## 2129	NA	0.73118513	-6.494707e-01	LYS	29.188956
## 2130	NA	0.75616802	-3.108319e-01	LYS	29.188956
## 2131	NA	0.60551211	-4.571685e-01	LYS	29.188956
## 2132	NA	0.65968754	-8.300068e-01	LYS	29.188956
## 2133	NA	0.72924047	-7.183200e-01	LYS	29.188956
## 2134	NA	0.56545159	-3.959284e-01	LYS	29.188956
## 2135	NA	0.56133464	-6.371782e-01	LYS	29.188956
## 2136	NA	0.76595426	-7.692942e-01	LYS	29.188956
## 2137	NA	0.87445368	-7.972428e-01	LYS	29.188956
## 2138	NA	0.61724246	1.176449e+00	LYS	29.188956

## 2139	NA 0.64176635	-1.980132e-01	LYS	29.188956
## 2140	NA 0.77623483	-3.947784e-02	LYS	29.188956
## 2141	NA 0.61518337	-1.758103e-01	HIS	32.023835
## 2142	NA 0.79342744	-6.536965e-01	HIS	32.023835
## 2143	NA 0.59135449	-4.527639e-01	HIS	32.023835
## 2144	NA 0.74347576	-6.541971e-01	HIS	32.023835
## 2145	NA 0.72370253	-4.911325e-01	HIS	32.023835
## 2146	NA 0.85058980	-3.481211e-01	HIS	32.023835
## 2147	NA 0.82247416	1.212591e-01	HIS	32.023835
## 2148	NA 0.77187095	-9.389258e-01	HIS	32.023835
## 2149	NA 0.79294564	-6.281378e-01	HIS	32.023835
## 2150	NA 0.78740047	-5.228844e-01	HIS	32.023835
## 2151	NA 0.79535949	-5.020302e-01	HIS	32.023835
## 2152	NA 0.81621546	3.626462e-01	HIS	32.023835
## 2153	NA 0.77926596	9.523972e-01	HIS	32.023835
## 2154	NA 0.77645476	-7.869178e-01	HIS	32.023835
## 2155	NA 0.82386204	-5.693314e-01	HIS	32.023835
## 2156	NA 0.81284555	-2.714968e-01	HIS	32.023835
## 2157	NA 0.78469251	-2.559779e-01	HIS	32.023835
## 2158	NA 0.75737907	-4.775872e-01	HIS	32.023835
## 2159	NA 0.72194994	-3.118648e-01	HIS	32.023835
## 2160	NA 0.76586610	-4.754002e-01	LYS	30.036167
## 2161	NA 0.73777568	-9.162160e-01	LYS	30.036167
## 2162	NA 0.62671009	1.790589e-01	LYS	30.036167
## 2163	NA 0.82518317	-3.163596e-01	LYS	30.036167
## 2164	NA 0.59623025	2.022305e-01	LYS	30.036167
## 2165	NA 0.78038162	-4.881864e-01	LYS	30.036167
## 2166	NA 0.77668860	-3.964455e-01	LYS	30.036167
## 2167	NA 0.67633813	-9.260576e-01	LYS	30.036167
## 2168	NA 0.74937005	-4.796917e-01	LYS	30.036167
## 2169	NA 0.78258918	6.758821e-01	LYS	30.036167
## 2170	NA 0.81449499	-3.661596e-01	LYS	30.036167
## 2171	NA 0.81960861	-3.273037e-01	LYS	30.036167
## 2172	NA 0.94726788	-3.859776e-01	LYS	30.036167
## 2173	NA 0.80083031	-6.891212e-01	LYS	30.036167
## 2174	NA 0.62066080	-1.236368e-01	LYS	30.036167
## 2175	NA 0.73306274	-3.004224e-01	LYS	30.036167
## 2176	NA 0.77388830	-1.569395e-01	LYS	30.036167
## 2177	NA 0.73935239	-4.567469e-01	LYS	30.036167
## 2178	NA 0.64602880	-5.768017e-01	LYS	28.147970
## 2179	3068514 0.76173486	-5.427268e-02	LYS	28.147970
## 2180	NA 0.65729868	-3.026486e-01	LYS	28.147970
## 2181	NA 0.54533168	-5.215560e-01	LYS	28.147970
## 2182	NA 0.83724715	-6.521100e-01	LYS	28.147970
## 2183	NA 0.61910417	4.983629e-02	LYS	28.147970
## 2184	NA 0.55246860	-3.930791e-01	LYS	28.147970
## 2185	NA 0.77536621	-5.034376e-01	LYS	28.147970
## 2186	NA 0.72216957	5.617334e-02	LYS	28.147970
## 2187	NA 0.82986604	-3.906353e-01	LYS	28.147970
## 2188	NA 0.76419613	-8.036491e-01	LYS	28.147970
## 2189	NA 0.73672082	-4.232325e-01	LYS	28.147970
## 2190	NA 0.84930670	-3.326381e-01	LYS	28.147970
## 2191	NA 0.73741029	-8.138319e-01	LYS	28.147970
## 2192	NA 0.73209967	8.270030e-05	LYS	28.147970

## 2193	NA	0.73832323	-5.167439e-02	LYS	28.147970
## 2194	NA	0.69329621	-4.051976e-01	LYS	28.147970
## 2195	NA	0.75613919	-9.490152e-01	LYS	28.147970
## 2196	NA	0.73756656	-2.964204e-01	LYS	28.147970
## 2197	NA	0.82353942	-7.345970e-02	LEU	25.601812
## 2198	NA	0.56220833	-6.783497e-01	LEU	25.601812
## 2199	NA	0.71111107	-4.411585e-01	LEU	25.601812
## 2200	NA	0.13707296	-1.401319e-01	LEU	25.601812
## 2201	NA	0.33998874	-2.604967e-01	LEU	25.601812
## 2202	NA	0.52406593	5.003258e-01	LEU	25.601812
## 2203	NA	0.18806540	4.489641e-01	LEU	25.601812
## 2204	NA	0.37792083	-1.550939e-01	LEU	25.601812
## 2205	NA	0.65061516	5.982278e-01	LEU	25.601812
## 2206	NA	0.62188020	-7.289090e-01	LEU	25.601812
## 2207	NA	0.52748477	1.356866e-01	LEU	25.601812
## 2208	NA	0.32351760	5.825965e-01	LEU	25.601812
## 2209	NA	0.86070886	-5.712454e-01	LEU	25.601812
## 2210	NA	0.68293372	1.577873e-02	LEU	25.601812
## 2211	NA	0.82210797	-5.947396e-01	LEU	25.601812
## 2212	NA	0.42946148	-3.394928e-01	LEU	25.601812
## 2213	NA	0.23132307	-2.008078e-01	LEU	25.601812
## 2214	NA	0.55834866	-1.304235e-01	LEU	25.601812
## 2215	1187444	0.64419694	5.333514e-01	PRO	22.655599
## 2216	NA	0.70852907	1.505067e+00	PRO	22.655599
## 2217	NA	0.42458276	1.973982e+00	PRO	22.655599
## 2218	NA	0.68288508	2.390982e+00	PRO	22.655599
## 2219	NA	0.62187956	1.016300e+00	PRO	22.655599
## 2220	NA	0.76818643	6.172633e-01	PRO	22.655599
## 2221	NA	0.61541586	7.504680e-01	PRO	22.655599
## 2222	NA	0.68994277	2.607557e-01	PRO	22.655599
## 2223	NA	0.77538440	-4.903094e-01	PRO	22.655599
## 2224	NA	0.69726719	1.498430e+00	PRO	22.655599
## 2225	NA	0.74804550	6.246822e-01	PRO	22.655599
## 2226	NA	0.58410928	3.799987e-01	PRO	22.655599
## 2227	NA	0.69307652	2.905344e-01	PRO	22.655599
## 2228	NA	0.55952100	5.641367e-01	PRO	22.655599
## 2229	NA	0.69581130	1.480576e+00	PRO	22.655599
## 2230	NA	0.57847536	9.357796e-01	PRO	22.655599
## 2231	NA	0.75317749	9.694823e-01	PRO	22.655599
## 2232	NA	0.80718841	1.525135e+00	PRO	22.655599
## 2233	NA	0.43793925	-1.098632e+00	LEU	19.381619
## 2234	NA	0.58172490	-5.982888e-01	LEU	19.381619
## 2235	NA	0.75254267	-7.918356e-01	LEU	19.381619
## 2236	NA	0.80995037	-1.035228e+00	LEU	19.381619
## 2237	NA	0.82270026	-8.065145e-01	LEU	19.381619
## 2238	NA	0.66508821	-5.335011e-01	LEU	19.381619
## 2239	NA	0.37229467	-7.753929e-01	LEU	19.381619
## 2240	NA	0.11633092	-1.232539e-01	LEU	19.381619
## 2241	NA	0.87892506	-8.939463e-01	LEU	19.381619
## 2242	NA	0.86885870	-8.985214e-01	LEU	19.381619
## 2243	NA	0.86086432	-9.932562e-01	LEU	19.381619
## 2244	NA	0.72365268	-8.702693e-01	LEU	19.381619
## 2245	NA	0.86642072	-1.119959e+00	LEU	19.381619
## 2246	NA	0.86582670	-8.904186e-01	LEU	19.381619

## 2247	NA 0.74078351	-9.218553e-01	LEU	19.381619
## 2248	NA 0.84067993	-5.914083e-01	LEU	19.381619
## 2249	NA 0.75251353	-4.569192e-01	LEU	19.381619
## 2250	NA 0.81059177	-8.622592e-01	GLY	15.975316
## 2251	NA 0.41264691	-1.774541e-01	GLY	15.975316
## 2252	NA 0.62804427	-8.471855e-01	GLY	15.975316
## 2253	NA 0.72546220	-8.874090e-01	GLY	15.975316
## 2254	NA 0.79722589	-9.326942e-01	GLY	15.975316
## 2255	NA 0.25326108	-3.207501e-01	GLY	15.975316
## 2256	NA 0.75258295	-9.340238e-01	GLY	15.975316
## 2257	NA 0.78615533	-8.149059e-01	GLY	15.975316
## 2258	36217 0.39421621	-1.199656e-01	GLY	15.975316
## 2259	NA 0.74099107	-6.903510e-01	GLY	15.975316
## 2260	NA 0.78799528	-8.041619e-01	GLY	15.975316
## 2261	NA 0.77473244	-2.407756e-01	GLY	15.975316
## 2262	NA 0.64826774	-7.770195e-01	GLY	15.975316
## 2263	NA 0.72316703	-4.560469e-01	GLY	15.975316
## 2264	NA 0.79503044	-1.346384e+00	GLY	15.975316
## 2265	NA 0.79419086	-5.994933e-05	GLY	15.975316
## 2266	NA 0.80439504	-7.520199e-01	GLY	15.975316
## 2267	NA 0.45855033	-1.395626e-01	GLY	15.975316
## 2268	NA 0.74447375	-8.052218e-01	PHE	13.120902
## 2269	NA 0.58876414	-7.716607e-01	PHE	13.120902
## 2270	NA 0.70426342	6.889854e-01	PHE	13.120902
## 2271	NA 0.69113974	-8.793559e-01	PHE	13.120902
## 2272	NA 0.28700994	-1.900148e-01	PHE	13.120902
## 2273	NA 0.71884378	-7.138662e-01	PHE	13.120902
## 2274	NA 0.75224796	-7.986935e-01	PHE	13.120902
## 2275	NA 0.59731848	-6.095014e-01	PHE	13.120902
## 2276	NA 0.29469063	-4.952606e-01	PHE	13.120902
## 2277	NA 0.32994407	-5.737787e-01	PHE	13.120902
## 2278	NA 0.79755457	-1.071210e+00	PHE	13.120902
## 2279	NA 0.46234508	-7.753909e-01	PHE	13.120902
## 2280	NA 0.66269453	-6.732495e-01	PHE	13.120902
## 2281	NA 0.83532930	-9.079559e-01	PHE	13.120902
## 2282	NA 0.68786877	-6.274888e-01	PHE	13.120902
## 2283	NA 0.80891095	-5.198277e-01	PHE	13.120902
## 2284	NA 0.84725767	-3.609827e-01	PHE	13.120902
## 2285	NA 0.82478125	-8.373535e-01	PHE	13.120902
## 2286	NA 0.76584886	7.745927e-01	THR	9.706648
## 2287	NA 0.87013570	2.113016e+00	THR	9.706648
## 2288	NA 0.88347621	-8.004611e-01	THR	9.706648
## 2289	NA 0.81387944	-5.074942e-01	THR	9.706648
## 2290	NA 0.70848239	-6.126984e-01	THR	9.706648
## 2291	NA 0.74089677	7.712806e-02	THR	9.706648
## 2292	NA 0.76663430	-8.199122e-01	THR	9.706648
## 2293	NA 0.72727712	-8.511174e-01	THR	9.706648
## 2294	NA 0.71998891	-8.788543e-01	THR	9.706648
## 2295	NA 0.73085664	-6.354497e-01	THR	9.706648
## 2296	NA 0.82136072	-1.154688e+00	THR	9.706648
## 2297	NA 0.94911814	-9.105565e-01	THR	9.706648
## 2298	NA 0.59160282	-4.600502e-01	THR	9.706648
## 2299	NA 0.78702094	-4.645111e-01	THR	9.706648
## 2300	NA 0.67669502	-6.386233e-01	THR	9.706648

## 2301	NA	0.84306672	-5.952030e-01	THR	9.706648
## 2302	NA	0.88522856	-9.403830e-01	THR	9.706648
## 2303	NA	0.84949515	-7.194495e-01	THR	9.706648
## 2304	NA	0.72062375	-7.152603e-01	THR	9.706648
## 2305	NA	0.78839390	-8.313249e-01	PHE	7.589467
## 2306	36218	0.81669428	-7.236023e-01	PHE	7.589467
## 2307	NA	0.41624090	-2.976271e-01	PHE	7.589467
## 2308	NA	0.76119721	-5.170965e-01	PHE	7.589467
## 2309	NA	0.71372115	-3.825008e-01	PHE	7.589467
## 2310	NA	0.72947613	-6.696792e-01	PHE	7.589467
## 2311	NA	0.84407924	-7.704640e-01	PHE	7.589467
## 2312	NA	0.83255681	-9.399475e-01	PHE	7.589467
## 2313	NA	0.82751619	-8.267315e-01	PHE	7.589467
## 2314	NA	0.95156882	-9.444008e-01	PHE	7.589467
## 2315	NA	0.85614382	-6.028130e-01	PHE	7.589467
## 2316	NA	0.88675016	-9.190659e-01	PHE	7.589467
## 2317	NA	0.80713150	-8.596441e-01	PHE	7.589467
## 2318	NA	0.76078140	-6.716848e-01	PHE	7.589467
## 2319	NA	0.80000273	-8.369378e-01	PHE	7.589467
## 2320	NA	0.78593914	-8.340620e-01	PHE	7.589467
## 2321	NA	0.84428246	-9.363494e-01	PHE	7.589467
## 2322	NA	0.83039803	-1.631642e-01	PHE	7.589467
## 2323	NA	0.82352180	-5.888074e-01	PHE	7.589467
## 2324	NA	0.80462752	-1.147427e+00	ASN	15.464820
## 2325	NA	0.86972715	-4.884711e-01	ASN	15.464820
## 2326	NA	0.91656395	1.413911e-01	ASN	15.464820
## 2327	NA	0.79253717	-6.655175e-01	ASN	15.464820
## 2328	NA	0.41274364	-9.531656e-01	ASN	15.464820
## 2329	NA	0.82072655	-5.638956e-01	ASN	15.464820
## 2330	NA	0.86446259	-9.790201e-01	ASN	15.464820
## 2331	NA	0.89068082	-9.581802e-01	ASN	15.464820
## 2332	NA	0.81162047	-9.506841e-01	ASN	15.464820
## 2333	NA	0.80789931	-8.371070e-01	ASN	15.464820
## 2334	NA	0.54525882	-6.608137e-01	ASN	15.464820
## 2335	NA	0.79709486	-1.157235e+00	ASN	15.464820
## 2336	NA	0.81687300	-1.129217e+00	ASN	15.464820
## 2337	NA	0.77446878	-1.010633e+00	ASN	15.464820
## 2338	NA	0.78874133	-5.926883e-01	ASN	15.464820
## 2339	NA	0.80404940	-1.153008e+00	VAL	13.214829
## 2340	NA	0.75039377	-7.085338e-01	VAL	13.214829
## 2341	NA	0.80925159	-4.652294e-01	VAL	13.214829
## 2342	NA	0.69324100	-8.155700e-01	VAL	13.214829
## 2343	NA	0.80123325	-1.533687e+00	VAL	13.214829
## 2344	NA	0.75094644	-1.235152e+00	VAL	13.214829
## 2345	NA	0.80002530	-1.516302e+00	VAL	13.214829
## 2346	NA	0.81895612	-8.013557e-01	VAL	13.214829
## 2347	NA	0.64953194	-3.472844e-01	VAL	13.214829
## 2348	NA	0.80656987	-2.099745e-01	VAL	13.214829
## 2349	NA	0.70869805	-2.868313e-01	VAL	13.214829
## 2350	NA	0.74029374	-6.037193e-01	VAL	13.214829
## 2351	NA	0.65140901	-8.659375e-01	VAL	13.214829
## 2352	NA	0.42718935	-6.180999e-01	VAL	13.214829
## 2353	NA	0.66444435	-9.698039e-01	VAL	13.214829
## 2354	NA	0.80659275	-1.018328e+00	VAL	13.214829

## 2355	NA	0.71042611	-1.324994e+00	VAL	13.214829
## 2356	NA	0.87542190	-1.085030e+00	VAL	13.214829
## 2357	NA	0.78157496	-1.092189e+00	VAL	13.214829
## 2358	NA	0.93273428	-1.351116e-01	VAL	15.446123
## 2359	NA	0.92781279	-5.394197e-02	VAL	15.446123
## 2360	NA	0.83542063	-8.850248e-01	VAL	15.446123
## 2361	NA	0.83513623	-6.162533e-01	VAL	15.446123
## 2362	NA	0.73692797	-1.167984e+00	VAL	15.446123
## 2363	NA	0.84051303	-8.233748e-01	VAL	15.446123
## 2364	NA	0.90633041	-6.677353e-01	VAL	15.446123
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## 2367	129144	0.68075078	-6.436794e-01	VAL	15.446123
## 2368	NA	0.51185045	-1.001762e+00	VAL	15.446123
## 2369	NA	0.74315834	-3.959630e-01	VAL	15.446123
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## 2371	NA	0.63312895	-3.841743e-01	VAL	15.446123
## 2372	NA	0.76380286	-2.210018e-01	VAL	15.446123
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## 2374	NA	0.72998313	-5.549904e-01	VAL	15.446123
## 2375	NA	0.78119206	-6.053753e-01	GLY	18.253573
## 2376	NA	0.69592523	-1.109396e+00	GLY	18.253573
## 2377	NA	0.78271120	-6.699721e-01	GLY	18.253573
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## 2379	NA	0.69852552	-1.112728e+00	GLY	18.253573
## 2380	NA	0.73567231	5.509644e-02	GLY	18.253573
## 2381	NA	0.80547249	-5.018210e-01	GLY	18.253573
## 2382	NA	0.84392452	-6.162645e-02	GLY	18.253573
## 2383	NA	0.74309022	7.176700e-01	GLY	18.253573
## 2384	NA	0.86274933	-6.981111e-01	GLY	18.253573
## 2385	NA	0.79357607	-7.519834e-01	GLY	18.253573
## 2386	NA	0.80471670	-1.452018e+00	GLY	18.253573
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## 2388	NA	0.83843829	-2.836712e-01	GLY	18.253573
## 2389	NA	0.81741847	-1.036714e+00	GLY	18.253573
## 2390	NA	0.58465452	-6.236846e-01	GLY	18.253573
## 2391	NA	0.87695614	2.311932e+00	GLY	18.253573
## 2392	NA	0.76376143	-4.857710e-01	GLY	18.253573
## 2393	NA	0.82584858	9.725628e-02	GLY	18.253573
## 2394	NA	0.81953199	-1.167964e+00	LEU	17.651889
## 2395	NA	0.75457545	-9.024797e-01	LEU	17.651889
## 2396	NA	0.82812373	-1.111837e+00	LEU	17.651889
## 2397	NA	0.81094700	-4.724185e-01	LEU	17.651889
## 2398	NA	0.82928983	2.331535e-01	LEU	17.651889
## 2399	NA	0.70548989	-8.374843e-01	LEU	17.651889
## 2400	NA	0.79448201	-9.283069e-01	LEU	17.651889
## 2401	NA	0.78570872	-1.460908e-01	LEU	17.651889
## 2402	NA	0.66889566	-2.374202e-01	LEU	17.651889
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## 2404	NA	0.80105659	-9.193968e-01	LEU	17.651889
## 2405	NA	0.87801158	-3.356921e-01	LEU	17.651889
## 2406	NA	0.74048104	-8.363116e-01	LEU	17.651889
## 2407	NA	0.76015480	-9.645766e-01	LEU	17.651889
## 2408	NA	0.90119774	-1.891487e+00	LEU	17.651889

## 2409	NA	0.54976669	-6.524255e-01	LEU	17.651889
## 2410	NA	0.73260074	-1.314686e+00	LEU	17.651889
## 2411	NA	0.69418618	-5.615331e-01	LEU	17.651889
## 2412	NA	0.21842600	-6.630477e-01	LEU	17.624475
## 2413	NA	0.61038155	-5.225363e-01	LEU	17.624475
## 2414	NA	0.24039280	-7.063394e-01	LEU	17.624475
## 2415	NA	0.29032224	-4.589781e-01	LEU	17.624475
## 2416	NA	0.71223807	-8.624119e-01	LEU	17.624475
## 2417	NA	0.28126262	-5.682173e-01	LEU	17.624475
## 2418	NA	0.62667569	-1.328719e+00	LEU	17.624475
## 2419	NA	0.55385018	-7.796966e-01	LEU	17.624475
## 2420	NA	0.79124520	-5.556511e-01	LEU	17.624475
## 2421	NA	0.66546899	-6.677446e-01	LEU	17.624475
## 2422	NA	0.24774261	2.929127e-01	LEU	17.624475
## 2423	NA	0.51860090	-5.861423e-01	LEU	17.624475
## 2424	NA	0.22392350	-4.766082e-01	LEU	17.624475
## 2425	NA	0.74016431	-3.307536e-01	LEU	17.624475
## 2426	NA	0.75971034	-4.580342e-01	LEU	17.624475
## 2427	NA	0.61913923	1.606574e-03	LEU	17.624475
## 2428	NA	0.14783104	1.213753e+00	LEU	17.624475
## 2429	NA	0.80306359	1.361250e+00	ARG	20.909894
## 2430	NA	0.74336030	-8.645976e-01	ARG	20.909894
## 2431	NA	0.58564089	-6.970216e-01	ARG	20.909894
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## 2440	NA	0.62531417	-8.175170e-01	ARG	20.909894
## 2441	NA	0.71185165	-7.191673e-01	ARG	20.909894
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## 2448	NA	0.17671698	-3.229881e-02	ASP	22.352405
## 2449	NA	0.78131384	-6.014150e-01	ASP	22.352405
## 2450	NA	0.70517015	3.397989e-02	ASP	22.352405
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## 2455	NA	0.60337510	-3.656712e-01	ASP	22.352405
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## 2457	NA	0.87865096	6.556208e-01	ASP	22.352405
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## 2484	NA	0.82600580	-1.126283e+00	ILE	23.253780
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## 2487	NA	0.48793735	-8.478282e-01	ILE	23.253780
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## 2490	NA	0.81929510	-8.198719e-01	ILE	23.253780
## 2491	NA	0.67494883	-6.943435e-01	ILE	23.253780
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## 2494	NA	0.39425089	-6.534805e-01	ILE	23.253780
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## 2498	NA	0.82560753	-9.290473e-01	ILE	23.253780
## 2499	NA	0.77888951	-7.273927e-01	ILE	23.253780
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## 2501	NA	0.36255344	-7.326076e-02	ILE	23.253780
## 2502	NA	0.82700495	-9.898445e-02	LYS	26.278991
## 2503	NA	0.76023878	1.636889e-01	LYS	26.278991
## 2504	NA	0.81922987	7.179436e-01	LYS	26.278991
## 2505	NA	0.67843667	-4.434389e-01	LYS	26.278991
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## 2508	NA	0.83094142	1.893298e-01	LYS	26.278991
## 2509	NA	0.74725537	2.419195e+00	LYS	26.278991
## 2510	2110197	0.71176806	6.687130e-01	LYS	26.278991
## 2511	NA	0.81153552	7.860370e-01	LYS	26.278991
## 2512	NA	0.73053276	-3.342498e-01	LYS	26.278991
## 2513	NA	0.80305675	-5.521483e-01	LYS	26.278991
## 2514	NA	0.75048294	8.830954e-01	LYS	26.278991
## 2515	NA	0.78892894	-4.365529e-01	LYS	26.278991
## 2516	NA	0.80544695	-5.165570e-01	LYS	26.278991

## 2517	NA	0.62832665	-4.078208e-01	LYS	26.278991
## 2518	NA	0.83974438	6.607615e-01	LYS	26.278991
## 2519	NA	0.59559075	3.849850e-01	ARG	27.197442
## 2520	NA	0.42366566	-2.408912e-01	ARG	27.197442
## 2521	NA	0.61305638	-8.306061e-01	ARG	27.197442
## 2522	NA	0.62453299	-7.985321e-01	ARG	27.197442
## 2523	NA	0.67498037	-5.589189e-01	ARG	27.197442
## 2524	NA	0.77846159	-1.229878e+00	ARG	27.197442
## 2525	NA	0.61573623	-1.007373e+00	ARG	27.197442
## 2526	NA	0.59202342	-5.754622e-01	ARG	27.197442
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## 2530	NA	0.42993906	-4.137088e-01	ARG	27.197442
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## 2533	NA	0.39413849	-7.488461e-01	ARG	27.197442
## 2534	NA	0.62300144	-5.365873e-01	ARG	27.197442
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## 2546	NA	0.17398333	8.592957e-02	ARG	28.194022
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## 2550	NA	0.74412979	-8.896918e-02	ARG	28.194022
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## 2571	NA 0.67038488	2.856130e-01	GLY	30.208751
## 2572	NA 0.63342418	-3.337856e-01	GLY	30.208751
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## 2576	NA 0.63979010	2.666536e-01	ASP	30.105425
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## 2579	NA 0.89648780	-6.809033e-03	ASP	30.105425
## 2580	NA 0.84499734	9.004769e-01	ASP	30.105425
## 2581	NA 0.76464205	-7.429365e-01	ASP	30.105425
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## 2589	NA 0.83639046	-3.310112e-01	ASP	30.105425
## 2590	NA 0.72791526	-3.628607e-01	ASP	30.105425
## 2591	NA 0.67016048	-6.647515e-01	ASP	30.105425
## 2592	NA 0.78176904	1.051532e+00	ASP	30.105425
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## 2605	Other
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## 2676          Other
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## 2685          Other
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## 2699          Other
## 2700          Other
## 2701          Other
## 2702          Other
## [ reached 'max' / getOption("max.print") -- omitted 4236 rows ]
```

```
table(merged_df_out$clinvar_clinical_significance)
```

```
##
##                benign      conflict  likely_pathogenic
##                6617         2         85                83
## likely_risk_allele  pathogenic      VUS
##                2         26        123
```

```
# 1. Set up
set.seed(123)
n_boot <- 1000
match_window <- 0.05
n_patho <- nrow(merged_df_out %>% filter(pathogenic_status == "Pathogenic"))

# 2. Get abundance/residuals from pten_patho
patho_df <- merged_df_out %>% filter(pathogenic_status == "Pathogenic") %>% dplyr::select(DMS_score_abun
patho_df$group <- "Pathogenic"

# 3. Bootstrap sampling from non-patho pool with abundance matching
non_patho_pool <- merged_df_out %>% filter(pathogenic_status != "Pathogenic")

nrow(non_patho_pool)
```

```
## [1] 6829
```

```

bootstrap_medians <- vector("numeric", length = n_boot)

# Pre-group non-patho pool into bins
non_patho_pool <- non_patho_pool %>%
  mutate(bin = cut(DMS_score_abundance, breaks = seq(-0.5, 2, by = match_window)))

# Bin pathogenic variants accordingly
patho_df <- patho_df %>%
  mutate(bin = cut(DMS_score_abundance, breaks = seq(-0.5, 2, by = match_window)))

# Create lookup table for fast sampling
bin_lookup <- split(non_patho_pool$residuals, non_patho_pool$bin)

# Bootstrap matrix
bootstrap_matrix <- matrix(NA, nrow = n_boot, ncol = n_patho)

for (i in 1:n_boot) {
  for (j in 1:n_patho) {
    bin_j <- patho_df$bin[j]
    candidates <- bin_lookup[[as.character(bin_j)]]
    if (!is.null(candidates) && length(candidates) > 0) {
      bootstrap_matrix[i, j] <- sample(candidates, 1)
    }
  }
}

# Summarize into a dataframe
boot_df <- data.frame(
  group = "Random abundance-matched",
  residuals = apply(bootstrap_matrix, 1, median, na.rm = TRUE) # Mean across matches per bootstrap
)

# Combine with patho residuals
plot_df <- bind_rows(
  patho_df %>% dplyr::select(group, residuals),
  boot_df
)

label_df <- plot_df %>%
  group_by(group) %>%
  summarise(
    n = n(),
    median_val = median(residuals),
    y_max = max(residuals),
    .groups = "drop"
  )

label_df <- label_df %>%
  mutate(n_label = case_when(
    group == "Random abundance-matched" ~ "bootstrapped 1000 times",
    TRUE ~ paste0("n = ", n)
  ))

```

```

# Plot
p_fast2 <- ggplot(plot_df, aes(x = group, y = residuals, fill = group)) +
  geom_violin(trim = FALSE, scale = "width", alpha = 0.8, color = NA) +
  geom_jitter(width = 0.15, size = 2, alpha = 0.7, color = "lightgrey") +
  stat_summary(fun = median, geom = "crossbar", width = 0.4, color = "black", fatten = 1) +
  stat_summary(fun = median, geom = "point", shape = 23, size = 2.5,
    fill = "black", color = "black", stroke = 0.7) +

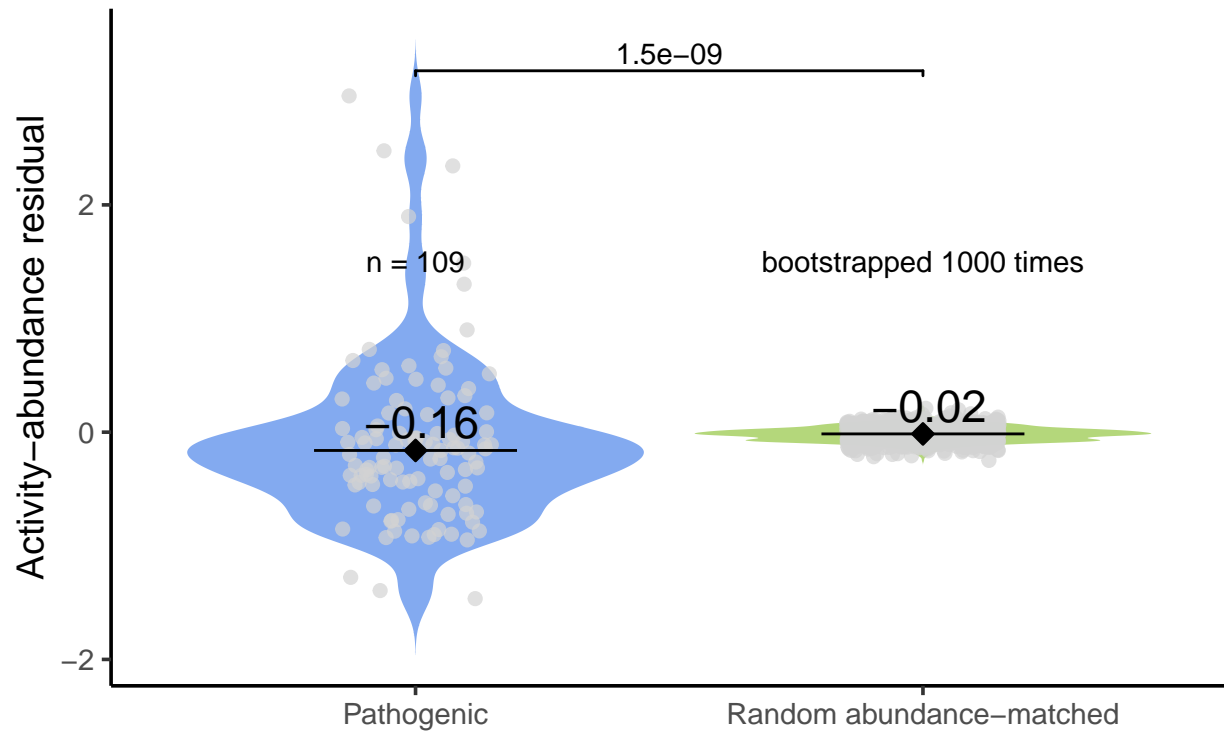
  geom_text(
    data = label_df,
    aes(x = group, y = 1.5, label = n_label),
    inherit.aes = FALSE,
    size = 4) +

  geom_text(
    data = label_df,
    aes(x = group, y = median_val + 0.25, label = sprintf(" %.2f", median_val)),
    inherit.aes = FALSE,
    size = 6
  ) +
  labs(
    x = "",
    y = "Activity-abundance residual",
    title = "Non-orthosteric variants"
  ) +
  theme_classic(base_size = 14) +
  scale_fill_manual(values = c("Pathogenic" = "cornflowerblue", "Random abundance-matched" = "darkolivegreen4"),
    legend.position = "none") +
  geom_signif(comparisons = list(c("Pathogenic", "Random abundance-matched")),
    map_signif_level = FALSE,
    test = "wilcox.test",
    tip_length = 0.01)

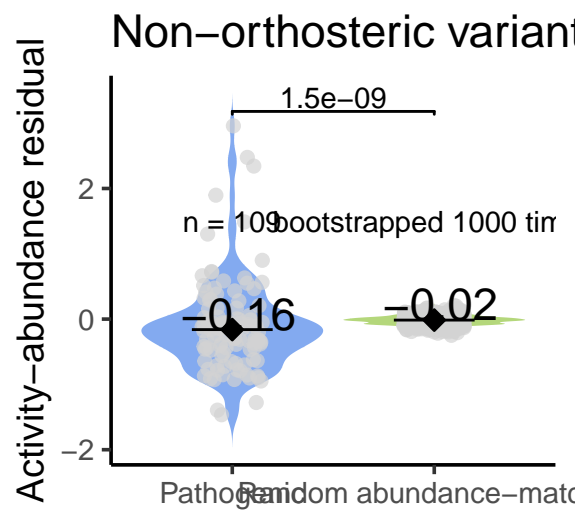
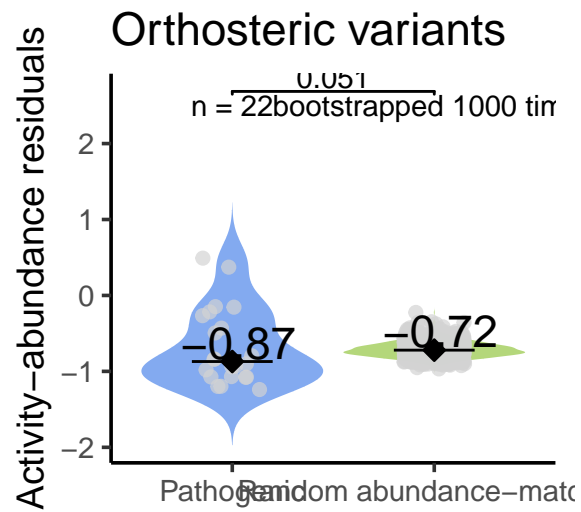
p_fast2

```


Non-orthosteric variants



```
fig5G<- plot_grid(p_fast, p_fast2, ncol=1, nrow=2)  
fig5G
```



```
ggsave("/Users/xl7/Documents/0.Projects/01.protein-seq-evo-v1/figs/panels/fig5_violin6.pdf",
  plot = fig5G, width = 3, height = 6, dpi = 300)
```