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Get Clearer Decomposition Results File

1. Open the _MMPBSA_info file in your Thai HPC HMG directory with your PBSA results:

   ```
   nano _MMPBSA_info
   ```

   ```
   # You can alter the variables below to change what info is printed out
   INPUT['debug_printlevel'] = 0
   INPUT['verbose'] = 1
   INPUT['csv_format'] = 1
   INPUT['dec_verbose'] = 3
   #
   ```

   Change ‘csv_format’ to 0 to make the readout easier to interpret

   Change ‘dec_verbose’ to 1

   Now, we can rewrite the output of the PBSA:

   ```
   load module Amber
   ```

   ```
   MMPBSA.py -rewrite-output
   ```

   If you use:

   ```
   cat FINAL_DECOMP_MMPBSA.dat
   ```

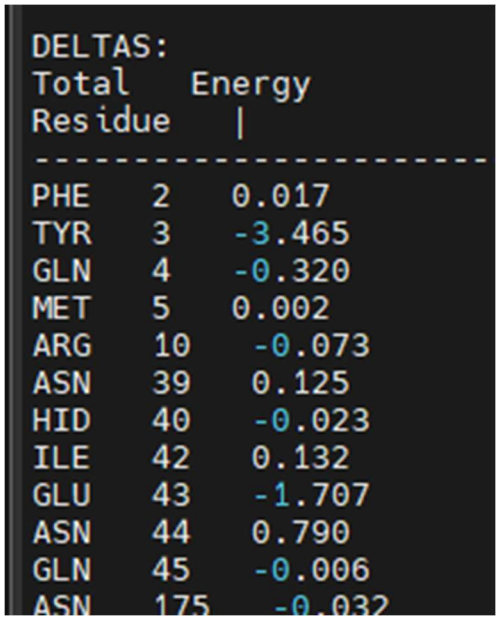
   you will see the data is presented nicer:

   ```
   DELTAS:
   Total Energy Decomposition:
   Residue | Location |      Internal      |    van der Waals    |    Electrostatic    |   Polar Solvation   |   Non-Polar Solv.   |       TOTAL
   ---------------------------------------------------------------------------------------------------------------------------------------------------
   PHE   2 | R PHE   2 |    0.000 +/-  0.000 |   -0.087 +/-  0.017 |    0.292 +/-  0.096 |   -0.188 +/-  0.097 |    0.000 +/-  0.000 |    0.017 +/-  0.057
   TYR   3 | R TYR   3 |    0.000 +/-  0.000 |   -3.735 +/-  0.409 |   -0.733 +/-  0.670 |    1.004 +/-  0.588 |    0.000 +/-  0.000 |   -3.465 +/-  0.544
   GLN   4 | R GLN   4 |    0.000 +/-  0.000 |   -0.286 +/-  0.069 |    0.054 +/-  0.202 |   -0.088 +/-  0.181 |    0.000 +/-  0.000 |   -0.320 +/-  0.105
   MET   5 | R MET   5 |    0.000 +/-  0.000 |   -0.039 +/-  0.010 |   -0.061 +/-  0.088 |    0.103 +/-  0.085 |    0.000 +/-  0.000 |    0.002 +/-  0.048
   ARG  10 | R ARG  10 |    0.000 +/-  0.000 |   -0.047 +/-  0.010 |    1.291 +/-  0.492 |   -1.317 +/-  0.588 |    0.000 +/-  0.000 |   -0.073 +/-  0.344
   ASN  39 | R ASN  39 |    0.000 +/-  0.000 |   -0.036 +/-  0.010 |   -0.109 +/-  0.078 |    0.271 +/-  0.204 |    0.000 +/-  0.000 |    0.125 +/-  0.195
   HID  40 | R HID  40 |    0.000 +/-  0.000 |   -0.035 +/-  0.010 |   -0.067 +/-  0.048 |    0.080 +/-  0.067 |    0.000 +/-  0.000 |   -0.023 +/-  0.058
   ```

   To extract this info:

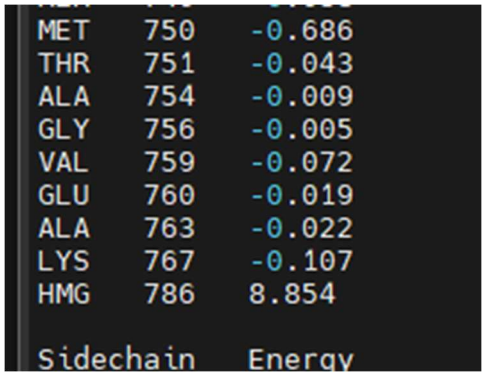
   ```
   awk '{print $1, " ", $2, " ", $28}' FINAL_DECOMP_MMPBSA.dat
   ```

   Scroll up to the ‘DELTAS’ information:



```
DELTAS:
Total   Energy
Residue   |
-----------------------
PHE   2   0.017
TYR   3   -3.465
GLN   4   -0.320
MET   5   0.002
ARG   10   -0.073
ASN   39   0.125
HID   40   -0.023
ILE   42   0.132
GLU   43   -1.707
ASN   44   0.790
GLN   45   -0.006
ASN   175   -0.032
```

Copy everything from PHE 2 to the end of these results



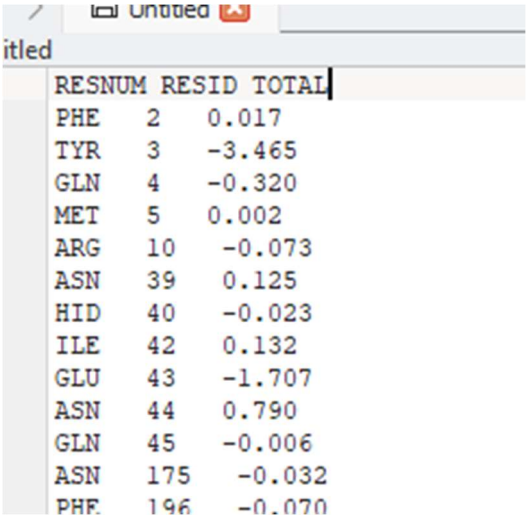
```
MET   750   -0.686
THR   751   -0.043
ALA   754   -0.009
GLY   756   -0.005
VAL   759   -0.072
GLU   760   -0.019
ALA   763   -0.022
LYS   767   -0.107
HMG   786   8.854

Sidechain   Energy
```

(Alternatively, you can save this to another file and open it in kate:

```
awk '{print $1, " ", $2, " ", $28}' FINAL_DECOMP_MMPBSA.dat > my_deltas.dat
```

)

Copy this into Kate and set the column names as decipted:



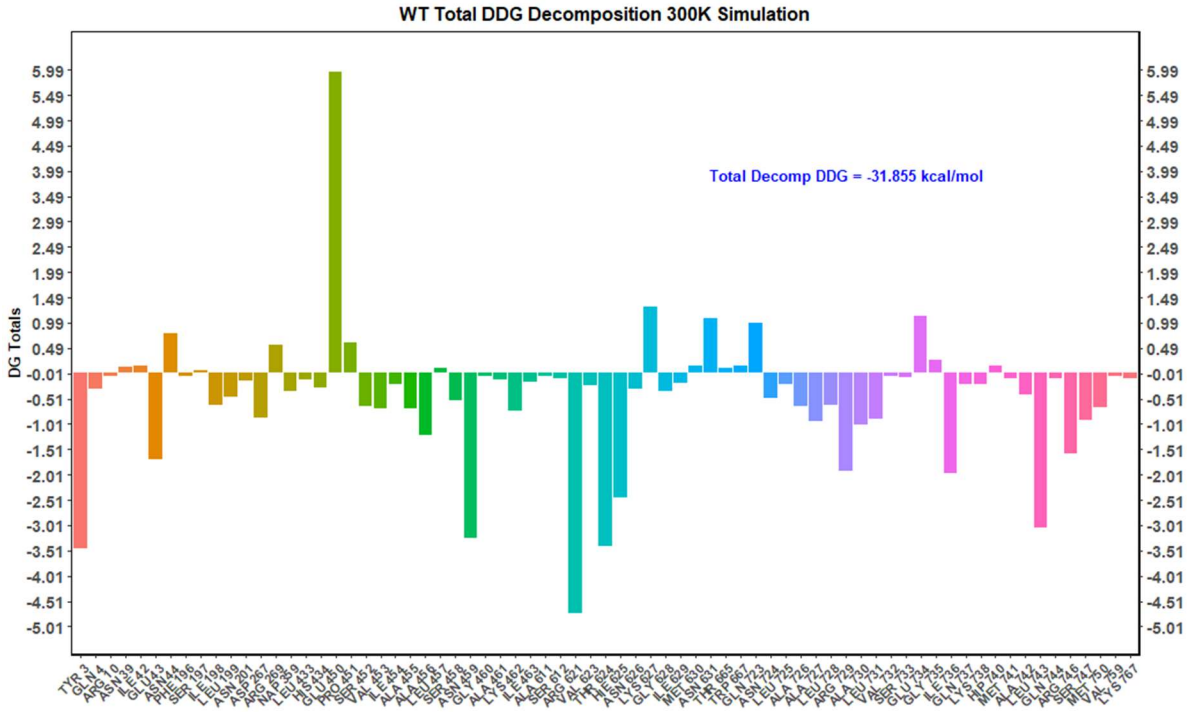
Save this as ‘decomp_deltas.dat’

The new Rscript reads this file along with the old files with some new lines:

```
decomp_deltas <- read.table('decomp_deltas.dat', header = TRUE, as.is=TRUE)

dg$TOTAL <- decomp_deltas$TOTAL
```

Here, all we’re doing is loading the new delta numbers file, and we are using the TOTAL values from it to overwrite the ones in our old decomposition file (which may have extracted the wrong values). This method is easier to verify that we successfully extracted the TOTALS from the dataframe. You should have both the ‘totals_ddg.dat’ and ‘decomp_deltas.dat’ in your folder that you’re running in R.

The new image puts on the total DDG from decomposition values present in the graph, but you could also change this to the MMGBSA values found in FINAL_MMPBSA_RESULTS.dat.


WT Total DDG Decomposition 300K Simulation
Total Decomp DDG = -31.855 kcal/mol
DG Totals
5.99
5.49
4.99
4.49
3.99
3.49
2.99
2.49
1.99
1.49
0.99
0.49
-0.01
-0.51
-1.01
-1.51
-2.01
-2.51
-3.01
-3.51
-4.01
-4.51
-5.01