INSTRUCTIONS FOR USING VMD SCRIPTS

http://niifhm.ru/wp-content/uploads/2015/04/VMD_script_for_describing_2_tetrad_GQs.txt

http://niifhm.ru/wp-content/uploads/2015/04/VMD_script_for_describing_3_tetrad_GQs.txt

http://niifhm.ru/wp-content/uploads/2015/04/VMD_script_for_describing_4_tetrad_GQs.txt

1) **Load a molecule of interest or a trajectory in VMD.**

For example, we load the 1KF1 directly from PDB by entering the accession code in the VMD molecule file browser form.

2) **Define the working folder on your PC in the VMD command window**

For example, the address of our working folder is "D:\parameters", so we type "cd D:\parameters", in the VMD command window.

3) **Download the appropriate script from our website and save it to your working folder.**

For example, 1KF1 is a 3-tetrad GQ, therefore, we go to http://niifhm.ru/wp-content/uploads/2015/04/VMD_script_for_describing_3_tetrad_GQs.txt and save the script as a text file to "D:\parameters".

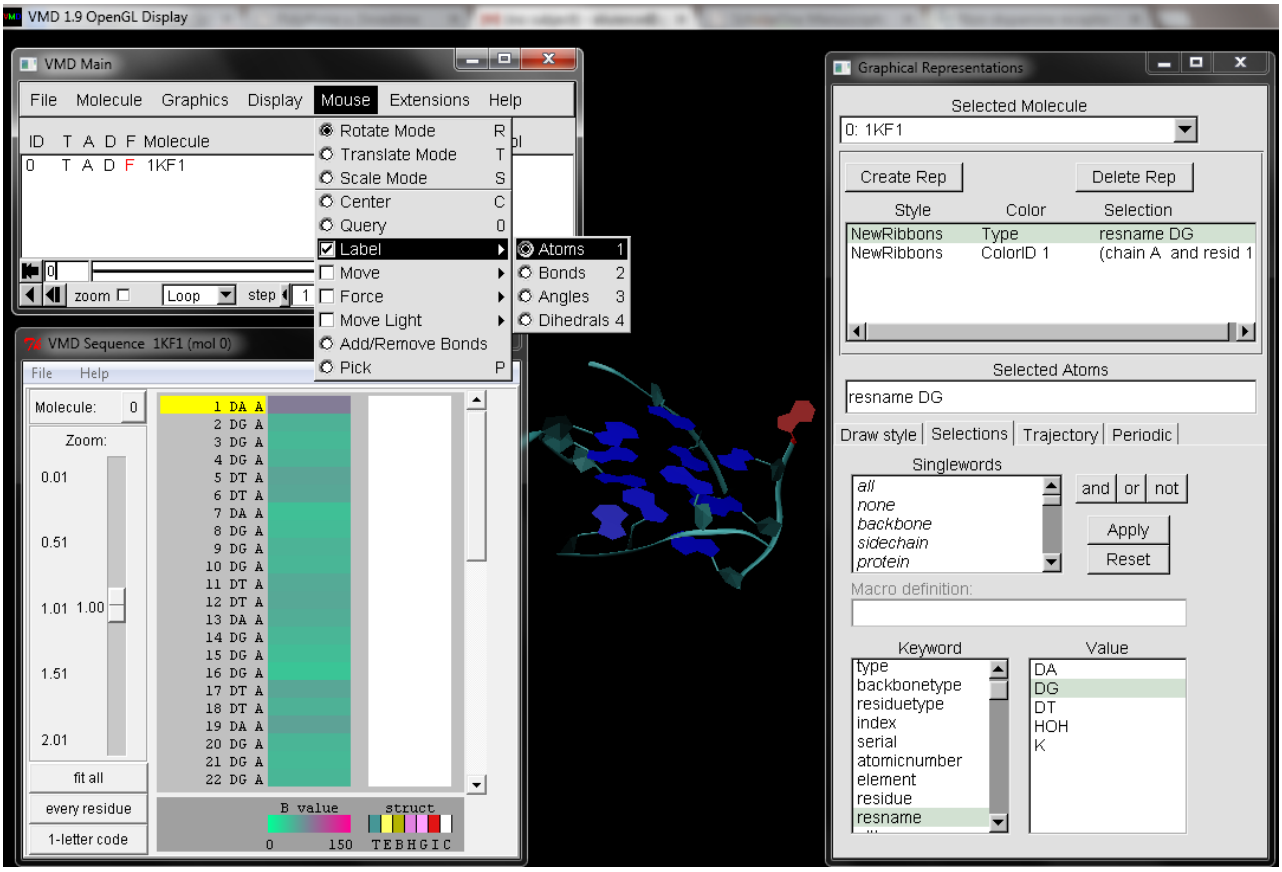
4) **Specify the molecule and set the correct numbers of Gua residues in your script file.**

This can be done in WordPad or any other suitable program. Below is the screenshot of the http://niifhm.ru/wp-content/uploads/2015/04/VMD_script_for_describing_3_tetrad_GQs.txt script, in which the ID numbers to be changed and the respective instructions in the headline are highlighted.

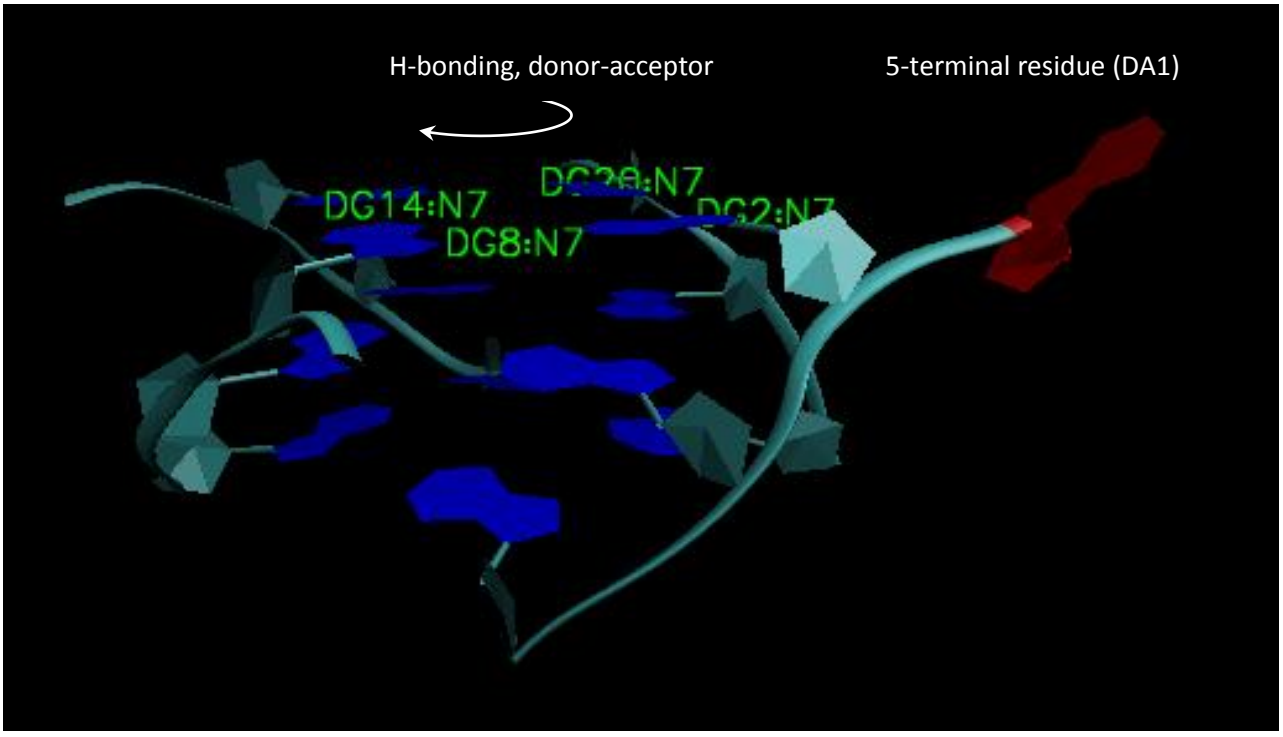
```
## Author: Tsvetkov V. B.
## v.b.tsvetkov@gmail.com
## The current script allows for calculation of the following parameters:
## q{alpha}q{beta}_r{alpha}i - angles between the normals to Gua planes in quartet {alpha} and
the axis of quartets {alpha} & {beta}
## q{alpha}_ij - angle between the normals to i & j Gua planes in quartet {alpha}
## q{alpha}_ij_kl and  q{alpha}_ijk_kli - angles between the nominal planes formed by Gua pairs
(i,j) & (k,l) or Gua triads (i,j,k) & (k,l,i) belonging to quartet {alpha}
## qr{alpha}i - distance between the quadruplex COM and the COM of Gua i belonging to quartet
{alpha}
## q{alpha}r{alpha}i - distance between the COM of quartet {alpha} and the COM of Gua i belonging
to quartet {alpha}
## q{alpha}q{beta} - distance between the COMs of quartets {alpha} & {beta}
## q{alpha}q{beta}t - twist angle for quartets {alpha} & {beta}
## rg_q - gyration radius of GQ
## rg_q{alpha} - gyration radius of quartet {alpha}
## r{alpha}ir{alpha}j - angle between the axes of guanines i & j in quartet {alpha}
## To use this script, one has to specify the molecule (set name_mol) and set the correct ID
numbers of Gua residues in the quartets (set nr{alpha}i, where i indicates Gua position in the
quartet and {alpha} is the quartet number)
set name_mol 2JSM
set nr11 3
set nr12 21
set nr13 17
set nr14 9
set nr21 4
set nr22 22
set nr23 16
set nr24 10
set nr31 5
set nr32 23
set nr33 15
set nr34 11
```

For example, to determine nr11-nr14 in VMD for the 1KF1 structure, we label the 5’-terminus, identify visually H-bonding direction in the 5’-teminal quartet and label Gua residues starting from the 5’-terminal one.

In the 1KF1snapshots below, GQ loops are hidden to provide a clear view on the GQ core.



1KF1 with labeled atoms in quartete1:



As evident from the snapshot, quartet 1 of the 1KF1 GQ is formed by the following residues: DG2: DG8: DG14: DG20 (from the 5'-terminus, donor→acceptor). Thus,
nr11 = 2,
nr12 = 8
nr13 = 14
nr14 = 20

Gua residues in quartets 2 and 3 are labeled accordingly, i.e., in the direction of H-bonding in quartet 1. Quartet 2 is DG3: DG9: DG15: DG21. Thus,
nr21 = 3,
nr22 = 9
nr23 = 15
nr24 = 21

Quartet 3 is DG4: DG10: DG16: DG22.
nr31 = 4,
nr32 = 10
nr33 = 16
nr34 = 22

We set these numbers in the script file and save all the changes (the final version with highlighted changes is shown below).

```
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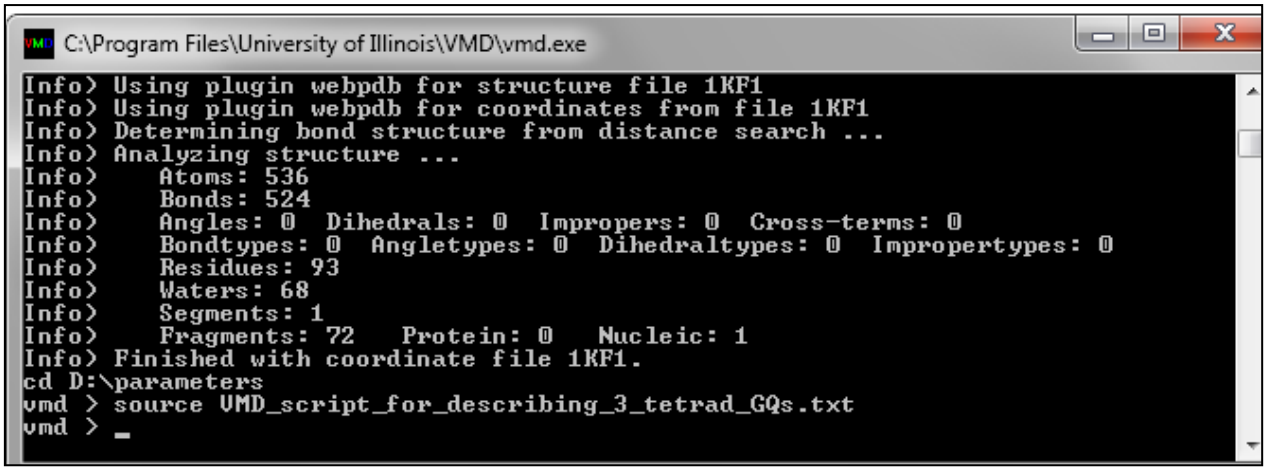
and the axis of quartets {alpha} & {beta}
## q{alpha}_ij - angle between the normals to i & j Gua planes in quartet {alpha}
## q{alpha}_ij_kl and  q{alpha}_ijk_kli - angles between the nominal planes formed by Gua
pairs (i,j) & (k,l) or Gua triads (i,j,k) & (k,l,i) belonging to quartet {alpha}
## qr{alpha}i - distance between the quadruplex COM and the COM of Gua i belonging to quartet
{alpha}
## q{alpha}r{alpha}i - distance between the COM of quartet {alpha} and the COM of Gua i
belonging to quartet {alpha}
## q{alpha}q{beta} - distance between the COMs of quartets {alpha} & {beta}
## q{alpha}q{beta}t - twist angle for quartets {alpha} & {beta}
## rg_q - gyration radius of GQ
## rg_q{alpha} - gyration radius of quartet {alpha}
## r{alpha}ir{alpha}j - angle between the axes of guanines i & j in quartet {alpha}
## To use this script, one has to specify the molecule (set name_mol) and set the ID numbers
of Gua residues in the quartets (set nr{alpha}i, where i indicates Gua position in the
quartet and {alpha} is the quartet number)
set name_mol 1KF1
set nr11 2
set nr12 8
set nr13 14
set nr14 20
set nr21 3
set nr22 9
set nr23 15
set nr24 21
set nr31 4
set nr32 10
set nr33 16
set nr34 22
set outfile1 [open ${name_mol}
_Quartet_1_Angles_between_the_normals_to_Gua_planes_and_the_axis_of_quartets_1_and_2.dat w]
puts $outfile1 [format "%4s\t%4s\t%4s\t%4s\t%4s\t" frame q1q2_r11 q1q2_r12 q1q2_r13 q1q2_r14]
set outfile2 [open ${name_mol}
_Quartet_2_Angles_between_the_normals_to_Gua_planes_and_the_axis_of_quartets_2_and_3.dat w]
puts $outfile2 [format "%4s\t%4s\t%4s\t%4s\t%4s\t" frame q2q3_r21 q2q3_r22 q2q3_r23 q2q3_r24]
set outfile3 [open ${name_mol}
_Quartet_3_Angles_between_the_normals_to_Gua_planes_and_the_axis_of_quartets_3_and_2.dat w]
puts $outfile3 [format "%4s\t%4s\t%4s\t%4s\t%4s\t" frame q3q4_r31 q3q4_r32 q3q4_r33 q3q4_r34]
set outfile5 [open ${name_mol}_Quartet_1_Angles_between_the_normals_to_Gua_planes.dat w]
puts $outfile5 [format "%4s\t%4s\t%4s\t%4s\t%4s\t%4s\t%4s\t" frame q1_12 q1_13 q1_14 q1_23
q1_24_c q1_34]
set outfile6 [open ${name_mol}_Quartet_2_Angles_between_the_normals_to_Gua_planes.dat w]
puts $outfile6 [format "%4s\t%4s\t%4s\t%4s\t%4s\t%4s\t%4s\t" frame q2_12 q2_13 q2_14 q2_23
q2_24_c q2_34]
set outfile7 [open ${name_mol}_Quartet_3_Angles_between_the_normals_to_Gua_planes.dat w]
puts $outfile7 [format "%4s\t%4s\t%4s\t%4s\t%4s\t%4s\t%4s\t" frame q3_12 q3_13 q3_14 q3_23
```

5) **Run the script from the VMD command window. The output files will be loaded into your working folder.**

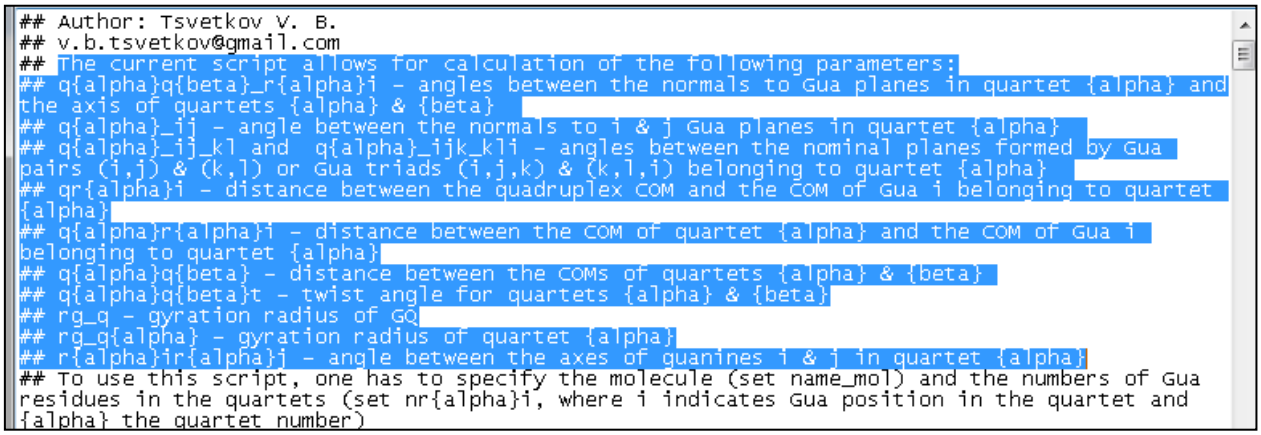
For example, we type “source VMD_script_fro_describing_3_tetrad_GQs.txt” in the command window.



In our working folder “parameters”, there are now 18 output files.

In the case of a 2-tetrad GQ, there would be 13 output files, and in the case of a 4-tetrad GQ – 23 files.

The contents of the output files in described in the script headline (see the highlighted section):



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## Author: Tsvetkov V. B.
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## The current script allows for calculation of the following parameters:
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## q{alpha}_ij - angle between the normals to i & j Gua planes in quartet {alpha}
## q{alpha}_ij_kl and  q{alpha}_ijk_kli - angles between the nominal planes formed by Gua
pairs (i,j) & (k,l) or Gua triads (i,j,k) & (k,l,i) belonging to quartet {alpha}
## qr{alpha}i - distance between the quadruplex COM and the COM of Gua i belonging to quartet
{alpha}
## q{alpha}r{alpha}i - distance between the COM of quartet {alpha} and the COM of Gua i
belonging to quartet {alpha}
## q{alpha}q{beta} - distance between the COMs of quartets {alpha} & {beta}
## q{alpha}q{beta}t - twist angle for quartets {alpha} & {beta}
## rg_q - gyration radius of GQ
## rg_q{alpha} - gyration radius of quartet {alpha}
## r{alpha}ir{alpha}j - angle between the axes of guanines i & j in quartet {alpha}
## To use this script, one has to specify the molecule (set name_mol) and the numbers of Gua
residues in the quartets (set nr{alpha}i, where i indicates Gua position in the quartet and
{alpha} the quartet number)
```

For example, our output file "1KF1_Quartet_2_Angles_between_the_normals_to_Gua_planes.dat"contains the following data:

frame	q2_12	q2_13	q2_14	q2_23	q2_24	q2_34
0	10.4355	15.9476	9.4101	11.7287	9.1195	6.7028

q2_ij is the angle between the normals to Gua_i and Gua_j in quartet 2.

If the initial pdb file contains several GQ models for the same sequence (as in the case of 2JSM), the output file will contain a respective number of rows: frames 0 – (X-1), where X is the number of models.

If the script is run for a trajectory, the output file will contain Y rows, where Y is the number of snapshots.