Computational Model and Dynamics of Monomeric Full-Length APOBEC3G

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Supporting Information

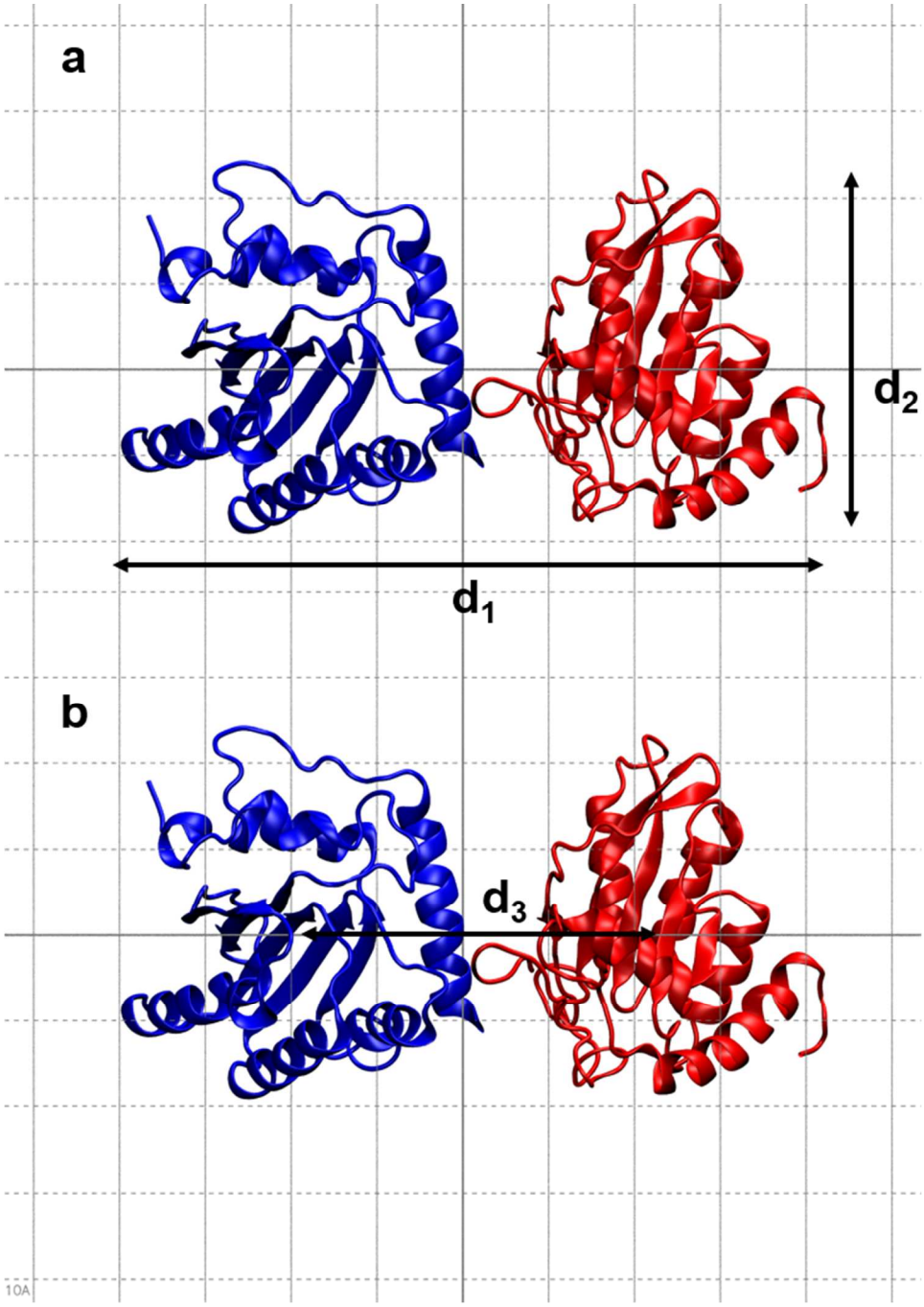

Figure S1. Representation of the defined spatial parameters, used in analyses of docked ensembles. (a) Parameters d_1 and d_2. (b) Parameter d_3. These parameters are defined in the methods section of the main text.

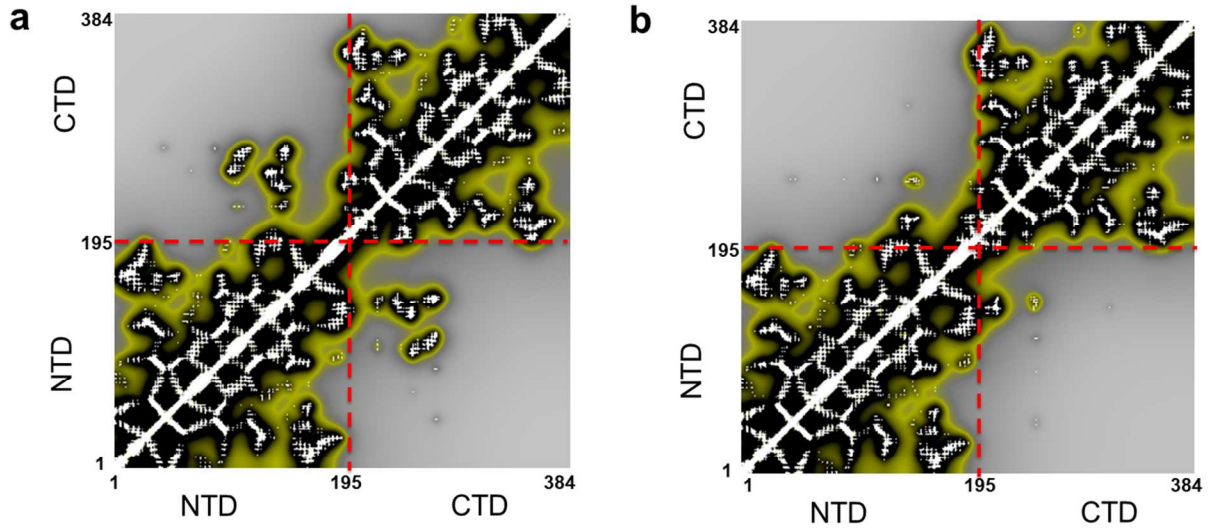

Figure S2. Protein residue-residue contact maps for a) dumbbell A3G structure, and b), globular A3G structure, obtained from 1μs MD simulation trajectories. The cutoff distance used in the contact map calculation is 1 nm.

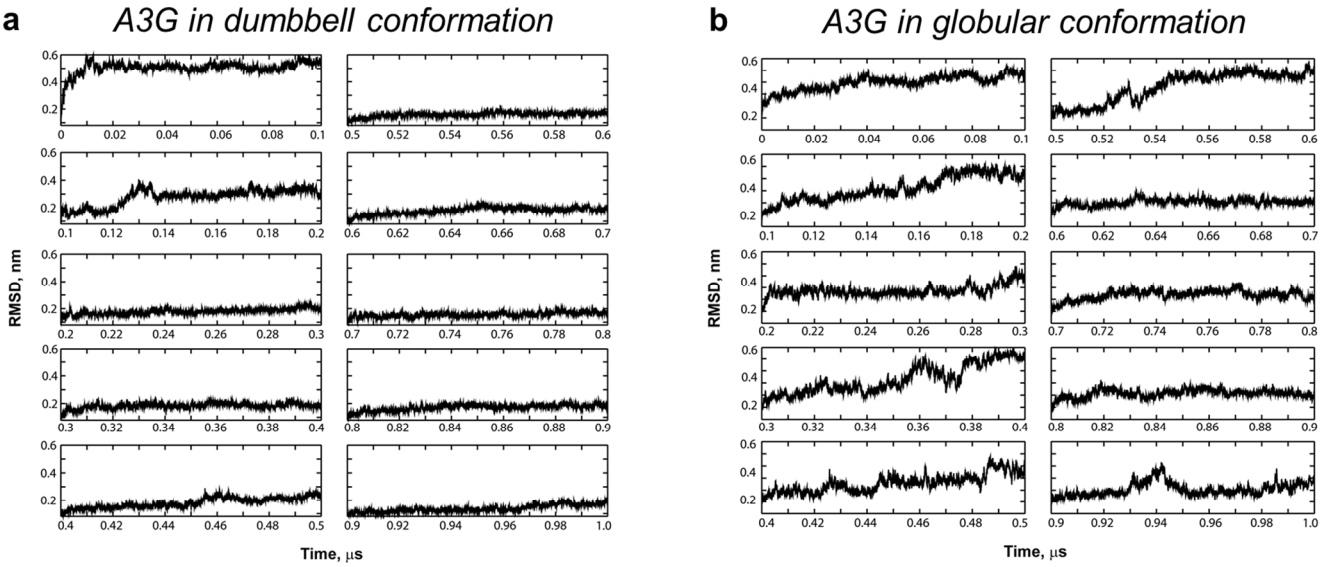

Figure S3. RMSD of A3G protein in a) dumbbell and b) globular conformations, calculated for partitioned 1 μs MD trajectories. Trajectories are partitioned into 100 ns long pieces, and RMSD plots are shown for each 100 ns piece, where the initial snapshot is used as a reference point.

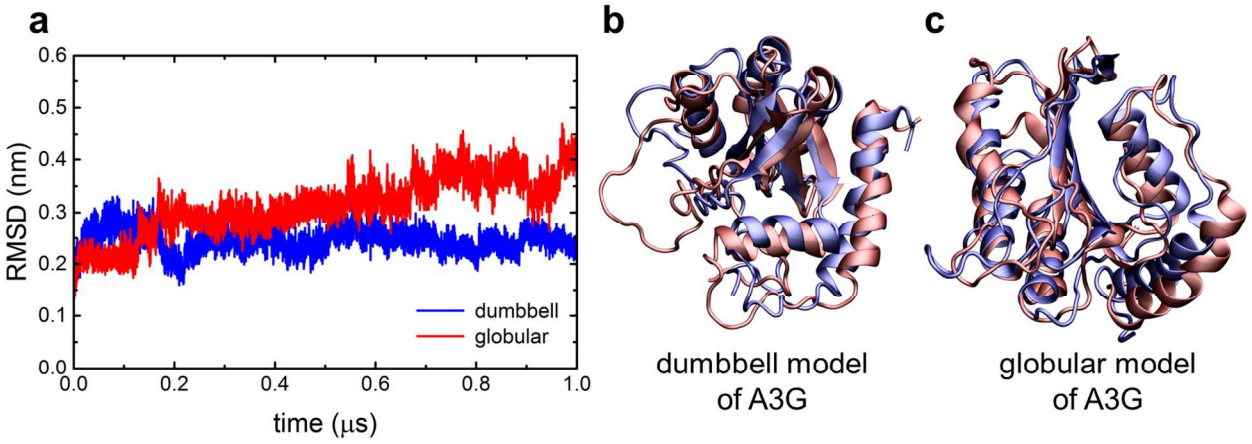

Figure S4. Conformational changes of A3G CTD in MD simulations. a) RMSD of CTD domains of A3G models in dumbbell and globular conformations. (b-c) Comparison of initial (blue) and final (red) conformations of CTD domains in dumbbell and globular shapes, obtained from 1 μs simulations. The alignment is performed on CTD regions with defined secondary structure (α-helices and β-sheets) for A3G residues 203-384.

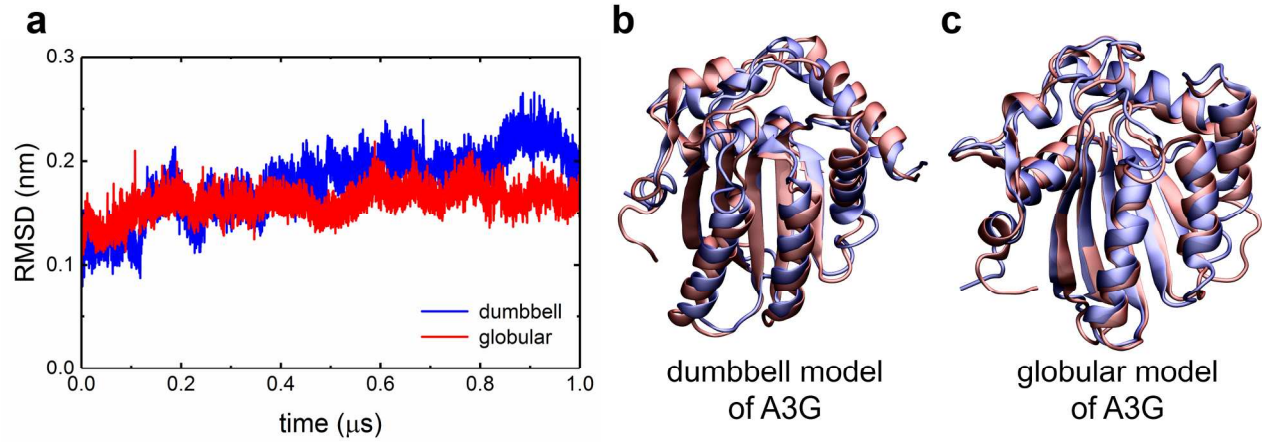

Figure S5. Conformational changes of A3G NTD in MD simulations. a) RMSD of NTD domains of A3G models in dumbbell and globular conformations. (b-c) Comparison of initial (blue) and final (red) conformations of NTD domains in dumbbell and globular shapes, obtained from 1 μs simulations. The alignment is performed on NTD regions with defined secondary structure (α-helices and β-sheets) for A3G residues 1-195.

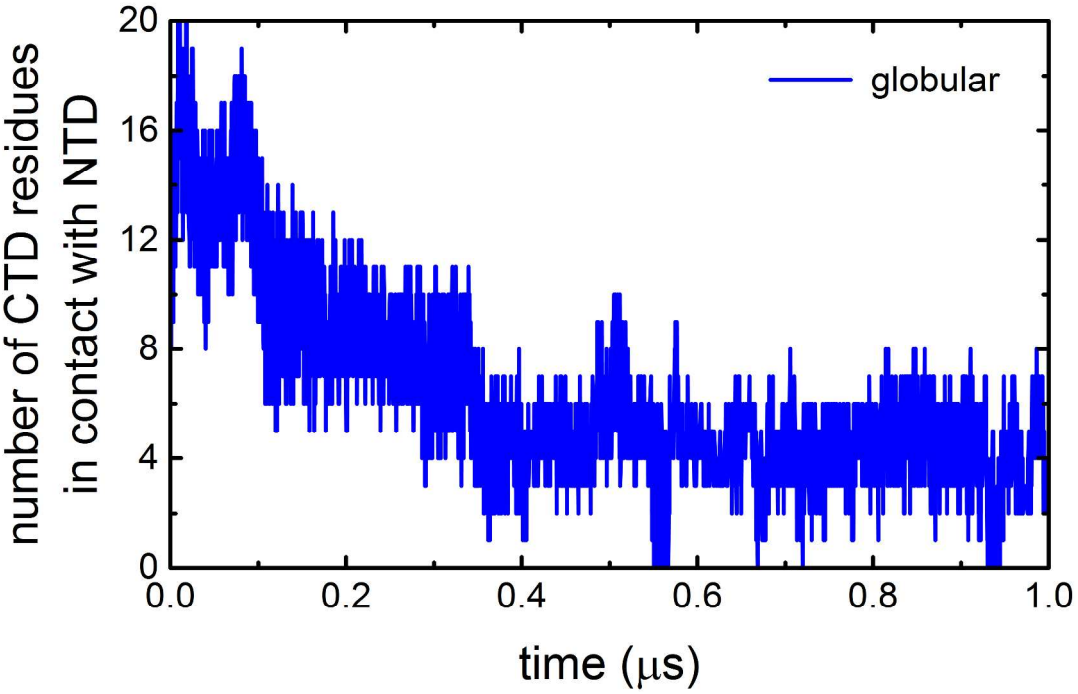

Figure S6. Number of CTD residues that are in contact with NTD of A3G monomer during A3G transition from globular to dumbbell conformation. The plot shows all the CTD residues (defined here as residues 203-384) that are within 3.5 Å of any NTD residue (defined here as residues 1-195).

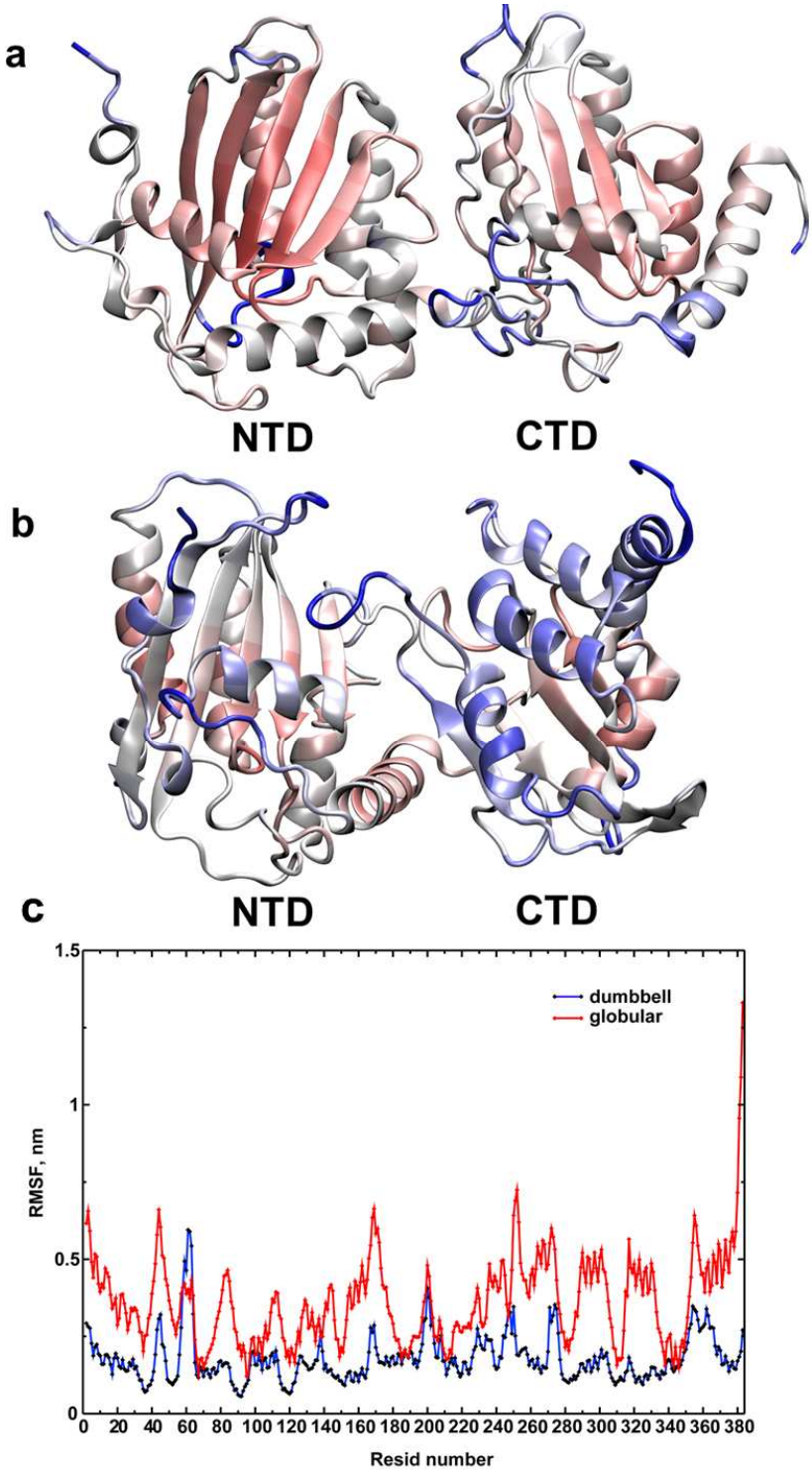

Figure S7. RMS fluctuations (RMSF) of A3G protein in dumbbell and globular conformations, calculated from 1 μs MD trajectories. RMSF values projected onto a) dumbbell and b) globular A3G structures. Red regions represent residues with small RMSF values, and blue regions represent residues with large RMSF values. c) RMSF plot for all residues of A3G in dumbbell and globular conformations.

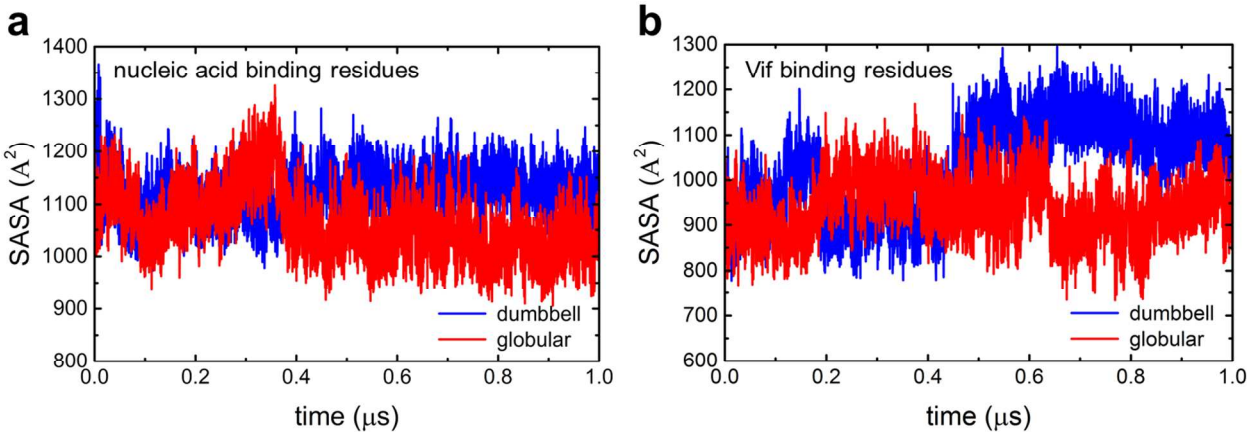

Figure S8. Time series of the solvent accessible surface area (SASA) of (a) nucleic acid and (b) Vif binding residues of A3G in globular and dumbbell conformations.

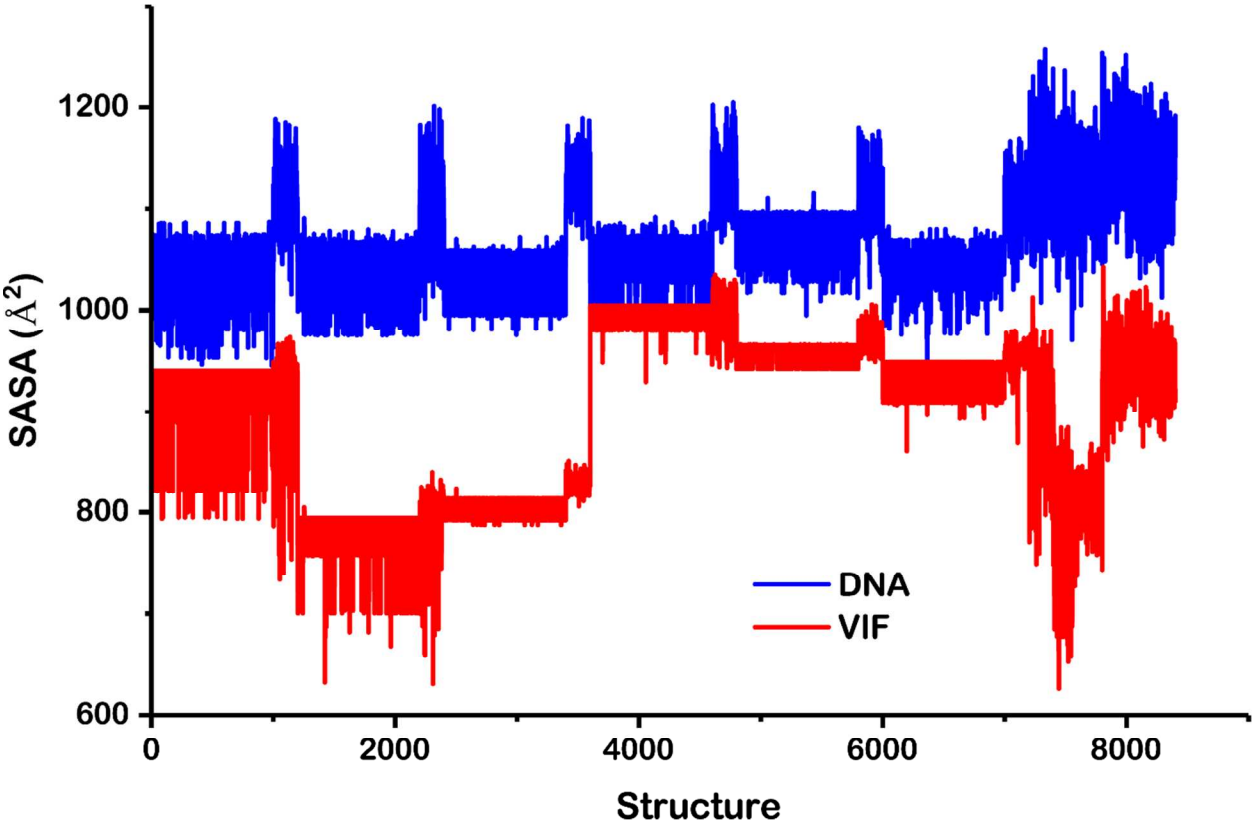

Figure S9. Solvent accessible surface area (SASA) of DNA (blue) and Vif (red) interacting amino acids of all the A3G complexes obtained from docking.

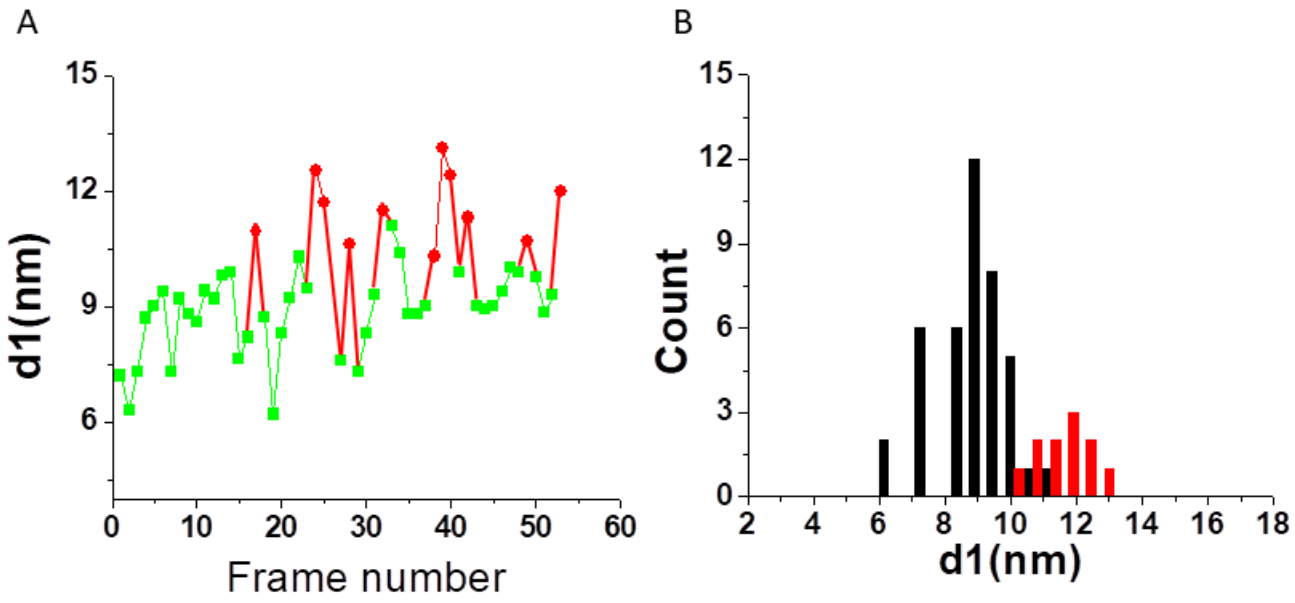

Figure S10. A) dependence of horizontal diameter d_1 for the globular and dumbbell structures on the frame number, obtained from one of the movies. Green squares and red circles correspond to globular and dumbbell conformations of A3G, respectively. Transitions from globular to the dumbbell structures are shown by the red lines. B) distribution of the globular (black bars) and dumbbell (red bars) structures of A3G.

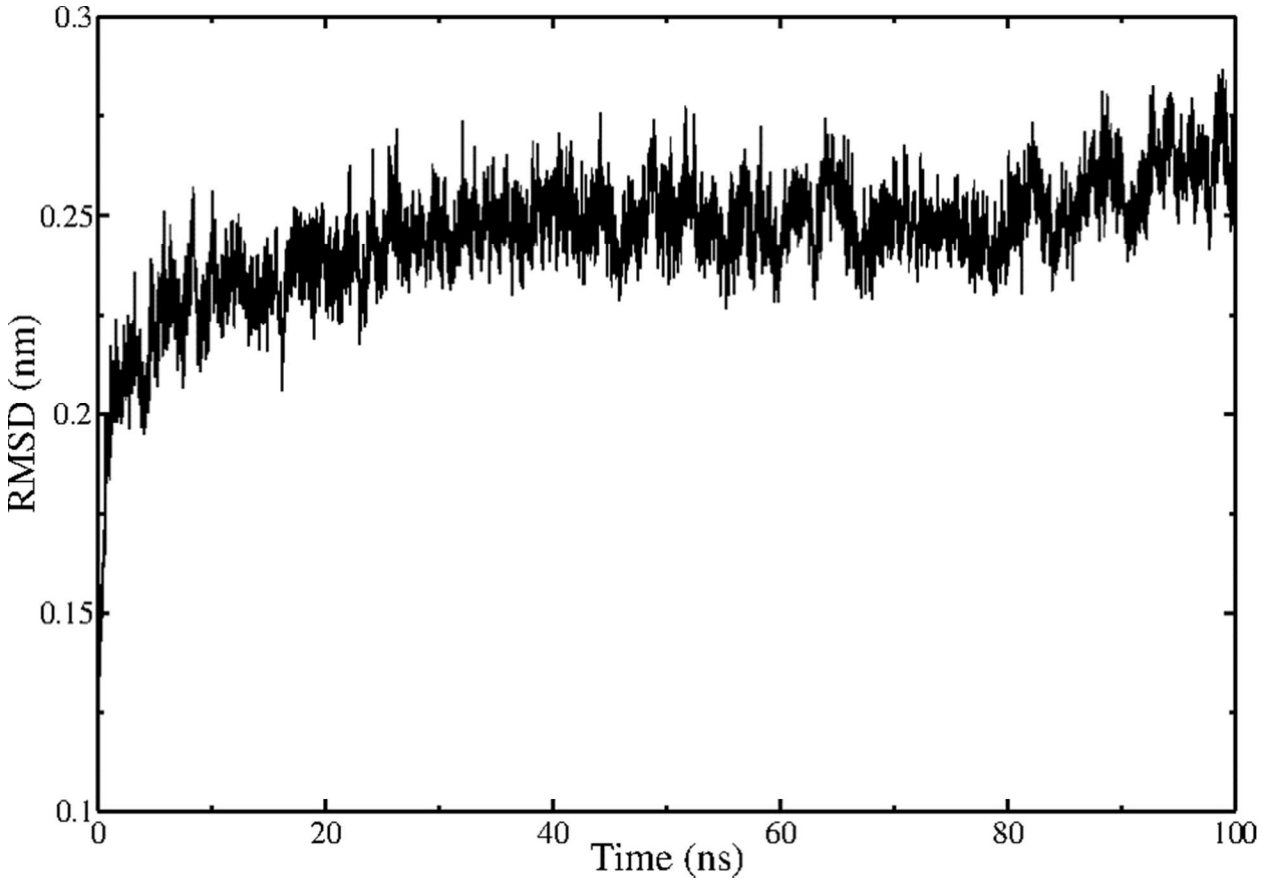

Figure S11. RMSD values of NTD domain during 100 ns molecular dynamics simulations

Supplementary Movie 1. Conformational transition of the representative globular form of a full A3G during a 1 μs MD trajectory. The flexible linker (residues 196-203), which repositions during the simulation course and correlates with the reorientation of two A3G domains, is shown as an orange tube. In the present movie, NTD domain of A3G is aligned with respect to its initial structure. NTD is shown in blue, and CTD is shown in red.

Supplementary Movie 2. Conformational transition of the representative globular form of a full A3G during a 1 μs MD trajectory. The flexible linker, which repositions during the simulation course and correlates with the reorientation of two A3G domains, is shown as an orange tube. In the present movie, CTD domain of A3G is aligned with respect to its initial structure. NTD is shown in blue, and CTD is shown in red.

Supplementary Movie 3. Initial fast transition of the DNA binding pocket from open state to transition state, as defined in the main text. In this transition, residue W94 is shown to change its position. The initial several nanoseconds of the 1 μs trajectory is shown for a representative dumbbell form of a full A3G. The residues W94 and Y124 are shown in green and yellow, respectively.

Supplementary Movie 4. Transition of the DNA binding pocket from transition state to the closed state, as defined in the main text. The trajectory shown includes the period from 400 ns to 600 ns, out of the total 1 μs MD trajectory of the A3G monomer in the dumbbell form. The residues W94 and Y124 are shown in green and yellow, respectively.

Supplementary Movie 5. Initial fast transition of the DNA binding pocket from open state to transition state, as defined in the main text. In this transition, residue W94 is shown to change its position. The initial several nanoseconds of the 1 μs trajectory is shown for a representative globular form of a full A3G. The residues W94 and Y124 are shown in green and yellow, respectively.

Supplementary Movie 6. Switching of the residue W94 from a transition state to a partially opening state of the representative globular form of a full A3G during a 1 μs MD trajectory. The residues W94 and Y124 are shown in green and yellow, respectively.

Supplementary Movie 7. High-speed AFM images illustrating dynamics of A3G monomer; the data were acquired with the rate 398 ms/frame.