

## SUPPORTING MATERIAL

### The systematic approach to describing conformational rearrangements in G-quadruplexes

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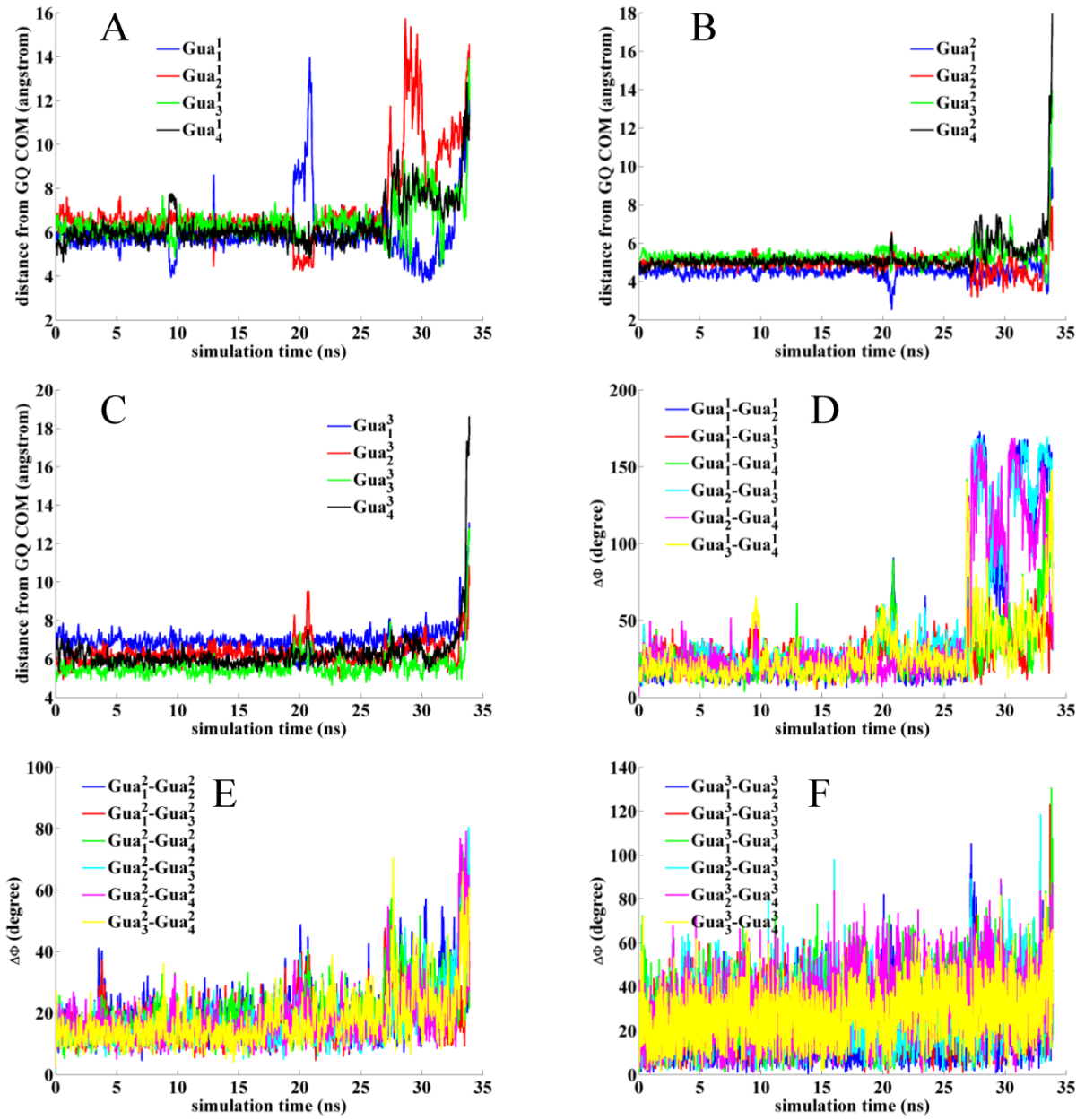
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**Table S1. Relative quartet positions in various types of GQs.**

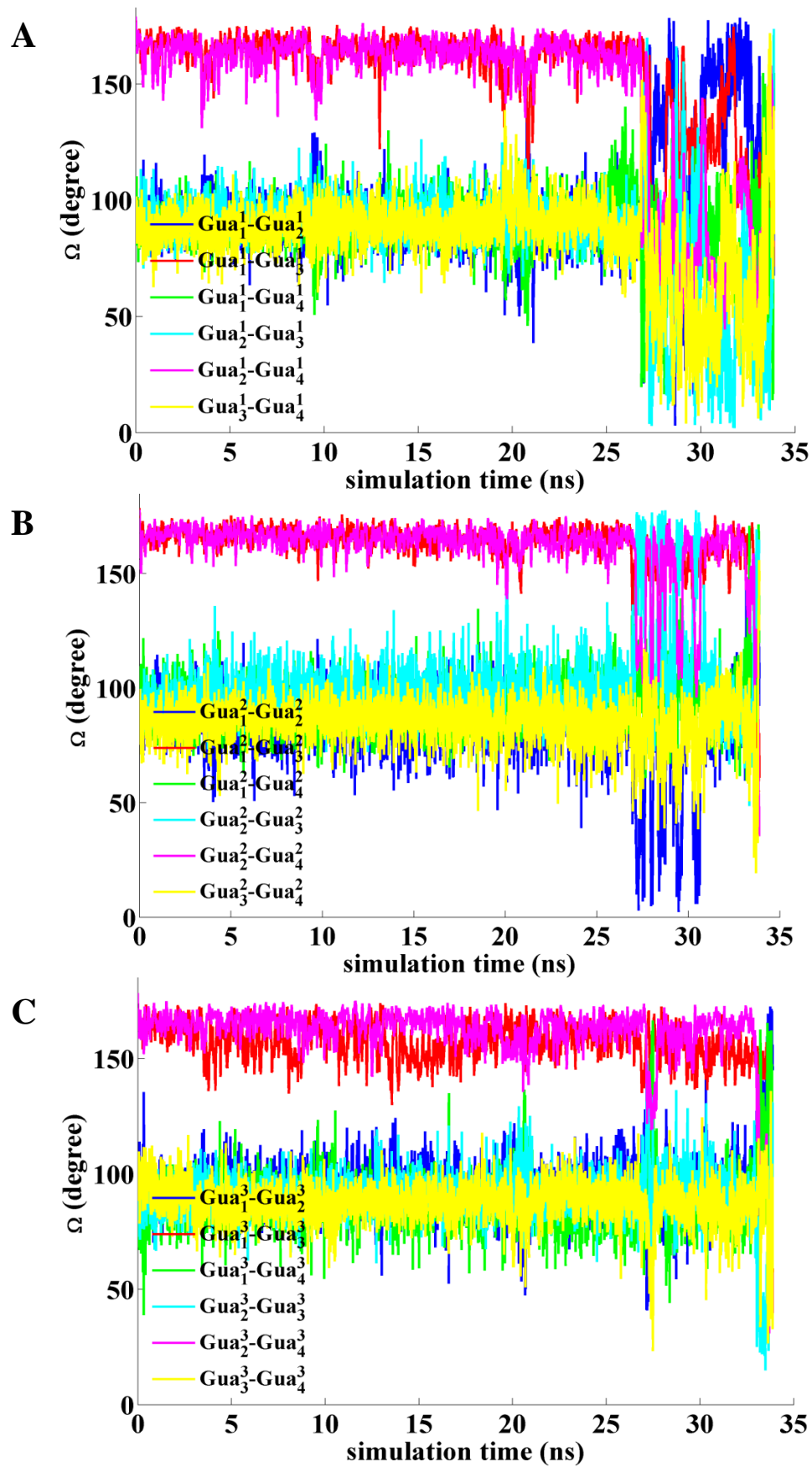
PDB entry	GQ description (number of tetrads, molecularity, folding type)	Quartets and their relative polarities <sup>a</sup>	Quartet COM dist., angstrom	Twist angle, degree
2JSM	Human telGQ hybrid 1 (3-tetrad, monomolecular, mixed)	1 and 2 - opposite	3.7	10
		2 and 3 - similar	3.9	23
1HAO	TBA GQ (2-tetrad, monomolecular, antiparallel)	1 and 2 - opposite	3.5	6
1HUT	TBA GQ (2-tetrad, monomolecular, antiparallel)	1 and 2 - opposite	3.5	9
1JPQ	Oxytricha telomeric GQ (4-tetrad, bimolecular, antiparallel)	1 and 2 - opposite	3.5	10
		2 and 3 - opposite	3.5	44
		3 and 4 - opposite	3.5	11
1KF1	Human telGQ in the presence of K <sup>+</sup> ions (3-tetrad, monomolecular, parallel)	1 and 2 - similar	3.4	28
		2 and 3 - similar	3.4	29
352D <sup>b</sup>	d(TG <sub>4</sub> T) <sup>b</sup> (4-tetrad, tetramolecular, parallel)	1 and 2 - similar	3.4	33
		2 and 3 - similar	3.3	28
		3 and 4 - similar	3.3	28

<sup>a</sup> Quartet numeration begins from the 5'-terminus. In the case of bimolecular/tetramolecular structures, it is the 5' terminus of strand 1 the PDB file.

<sup>b</sup> Two distinct stacking arrangements are noted for GQ. COM distances and the twist angles in the table represent average values.

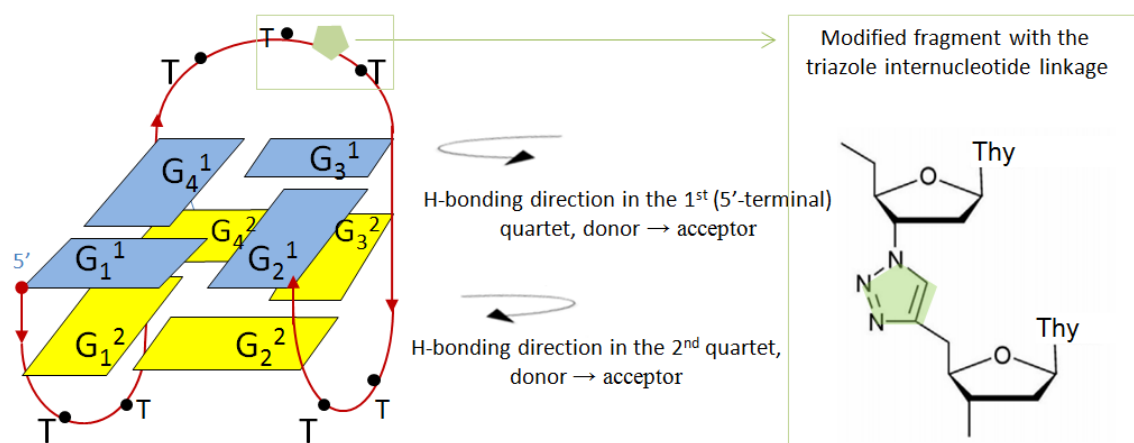


**Figure S1. Quartet integrity (A-C) and planarity (D-F) in telGQ.** A: Distances between the telGQ and Gua<sub>1</sub><sup>1</sup>-Gua<sub>4</sub><sup>1</sup> COMs; B: distances between the telGQ and Gua<sub>1</sub><sup>2</sup>-Gua<sub>4</sub><sup>2</sup> COMs; C: distances between the telGQ and Gua<sub>1</sub><sup>3</sup>-Gua<sub>4</sub><sup>3</sup> COMs. D: Angles between the normals to the Gua planes in quartet 1; E: angles between the Gua planes in quartet 2; F: angles between the Gua planes in quartet 3.

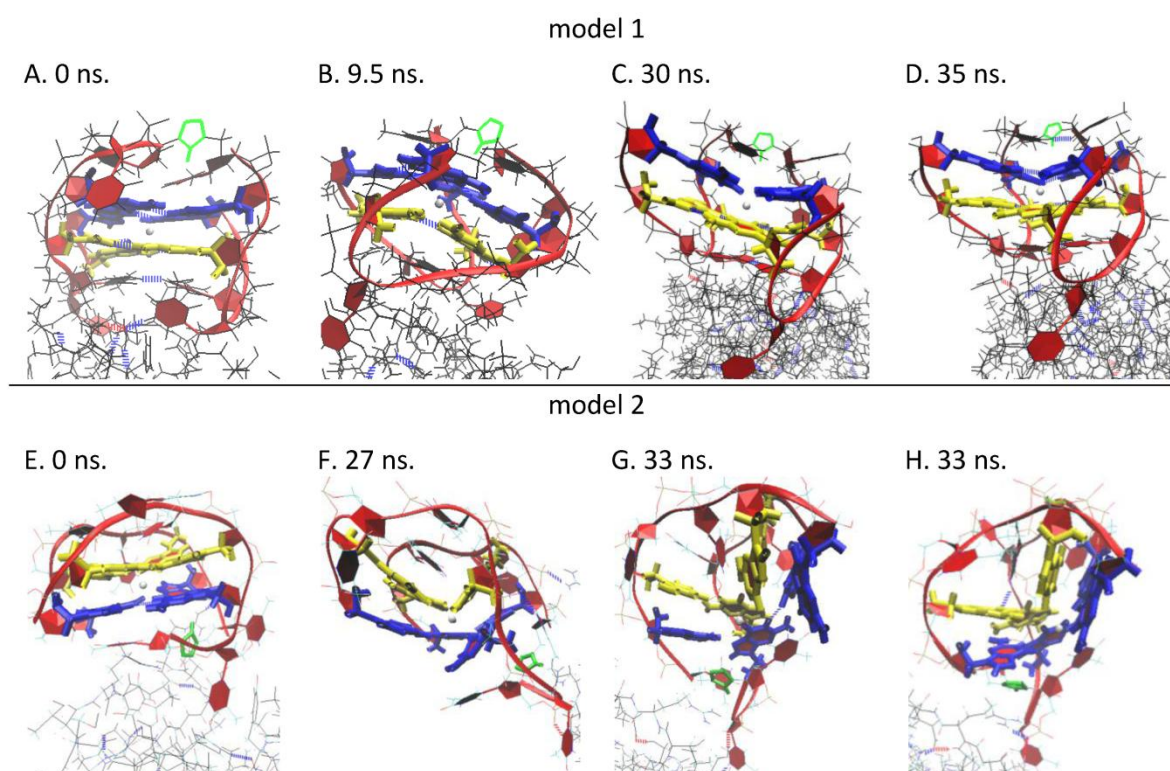


**Figure S2. Relative Gua rotation in telGQ.** A: Quartet 1; B: Quartet 2; C: Quartet 3.

## Triazole-TBA – schematic representation

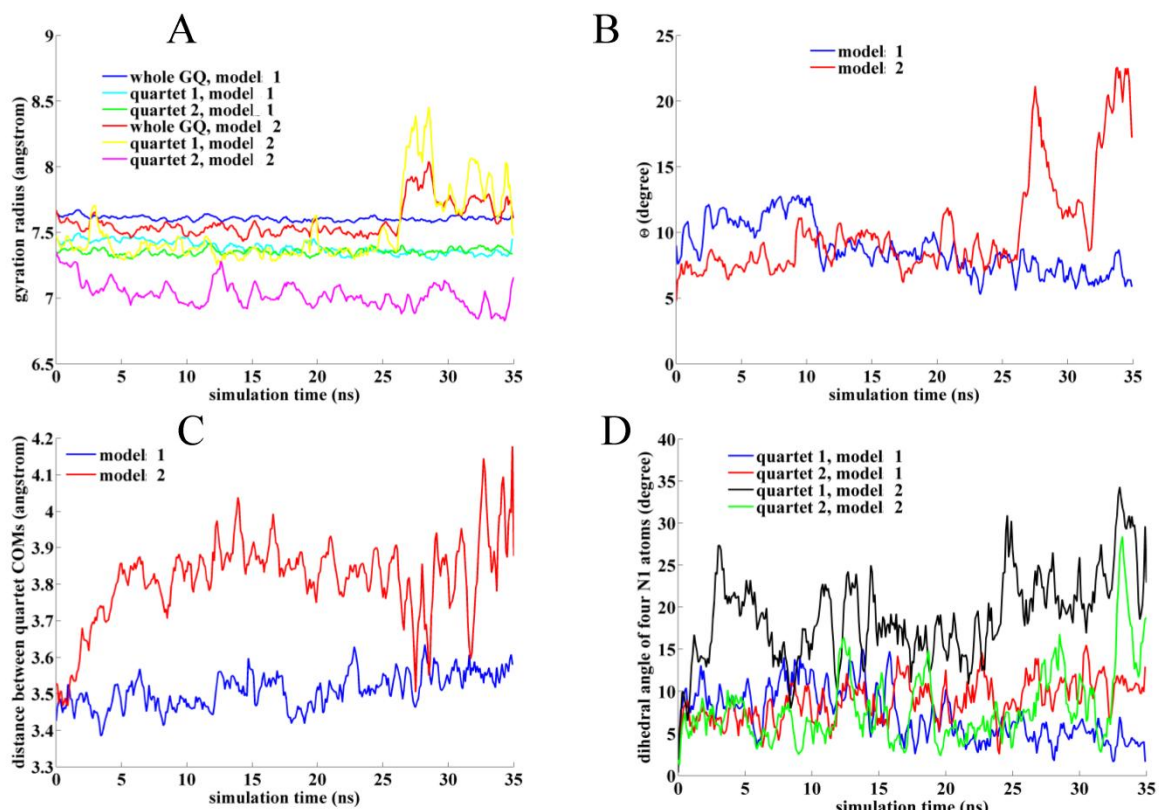


## MD snapshots

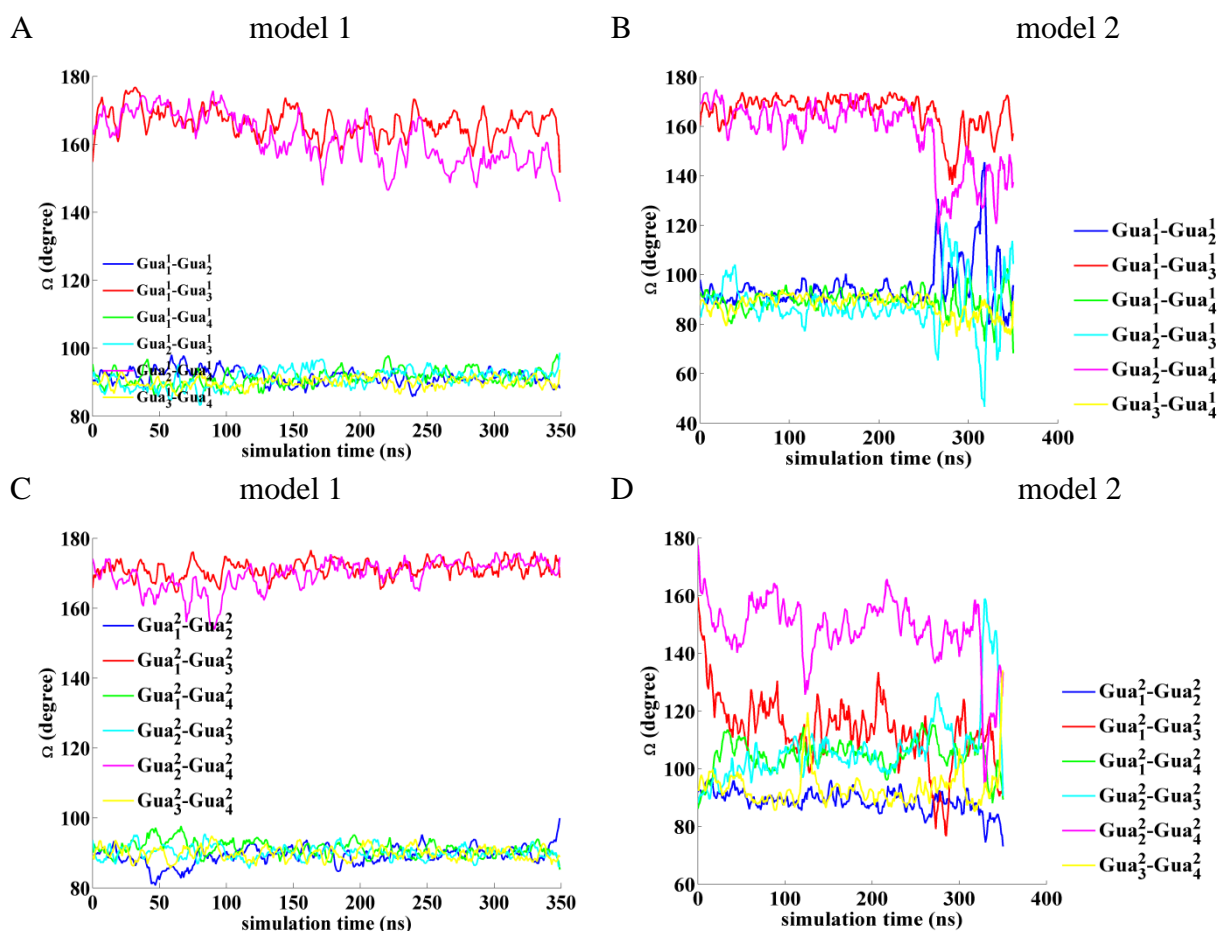


**Figure S3. Triazole-TBA and MD simulation snapshots for its complex with thrombin.**

Quartet 1 is blue; quartet 2 is yellow. The triazole fragment in the modified internucleotide linkage is green. A: Model 1 at 0 ns. The quartets are intact and parallel. B: Model 1 at 9.5 ns. Insignificant "lateral" bending in quartet 2. C: Model 1 at 30 ns. Insignificant "lateral" bending in quartet 1. D: Model 1 at 35 ns. The quartet 1 lateral bending was maintained. However, the GQ core was generally intact, and the bonds with thrombin were retained. E: Model 2 at 0 ns. The quartets are intact and parallel. F: Model 2 at 27 ns. The beginning of major GQ distortions. Gua<sub>2</sub><sup>1</sup> and Gua<sub>3</sub><sup>1</sup> deviate from quartet 1. Gua<sub>3</sub><sup>2</sup> deviates from quartet 2. G: Model 2 at 33 ns. Profound "lateral" bending in quartets 1 and 2. H: Quartets 1 and 2 maintain "lateral" bending. Most of the binding contacts with the protein were not retained.

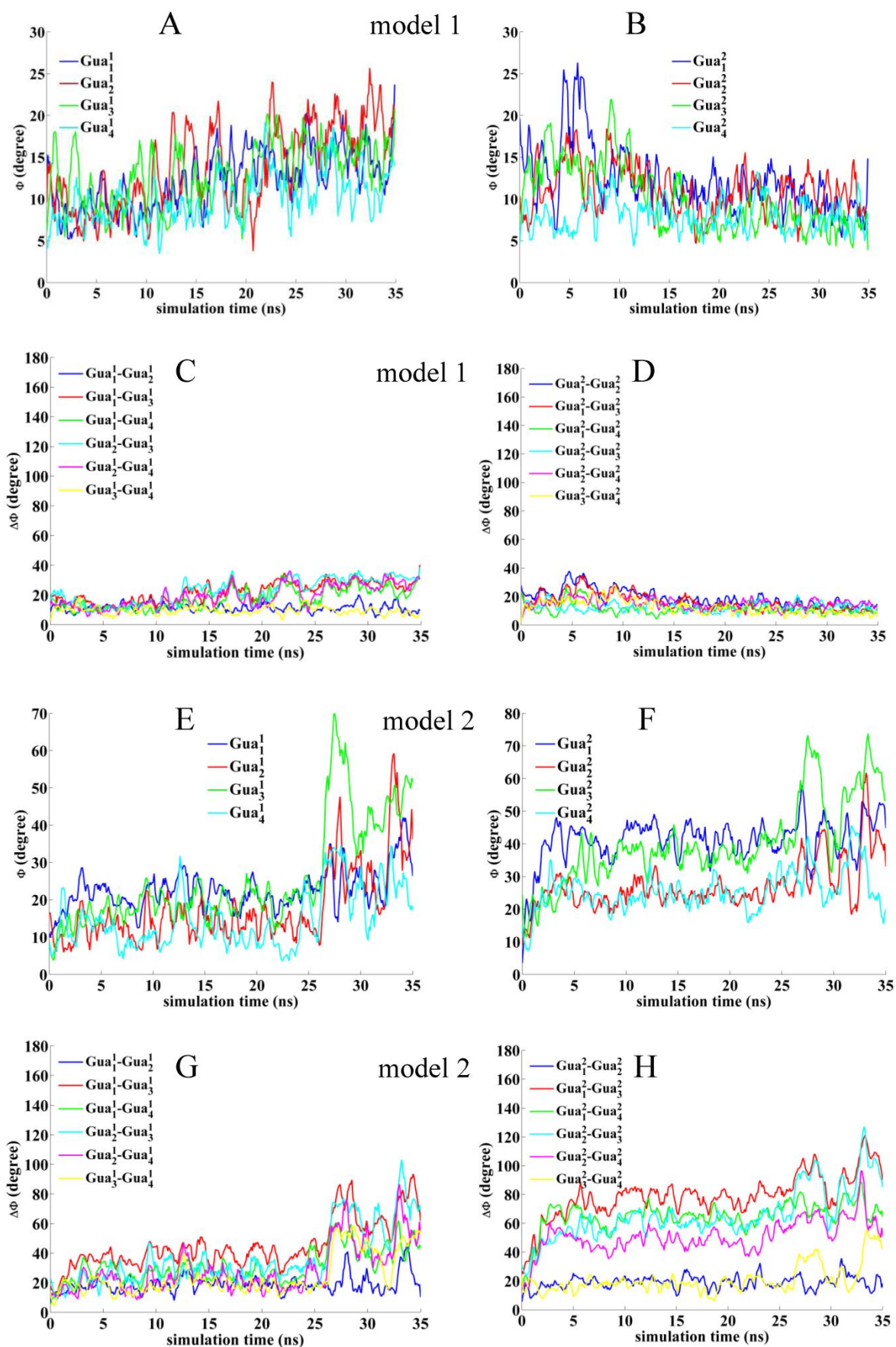


**Figure S4. Basic GQ-related parameters and their fluctuations during triazole-TBA MD simulation.** A: gyration radii; B: twist angles; C: distances between quartet COMs; D: the dihedral angles of the N1 atoms in each of the two quartets.



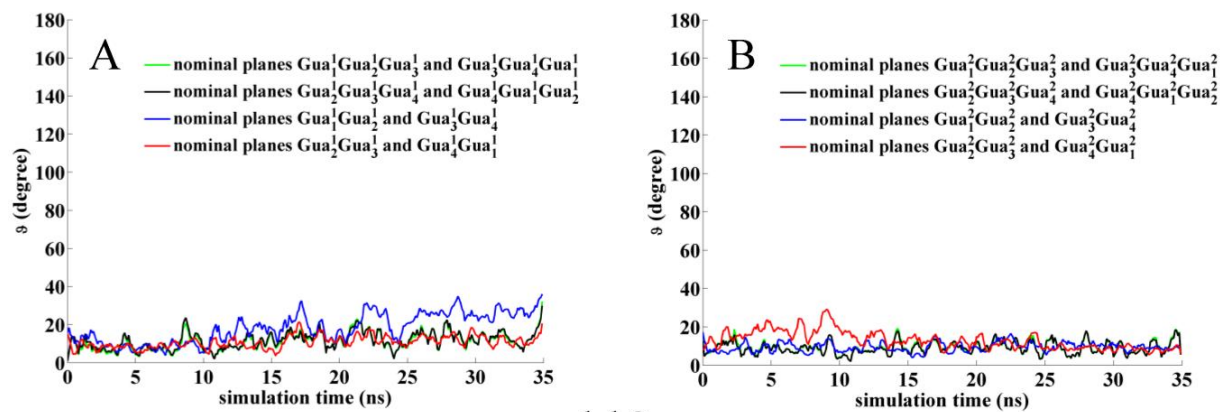
**Figure S5. Relative Gua rotation in the triazole-TBA quartets 1 (A and C) and 2 (B and D)**



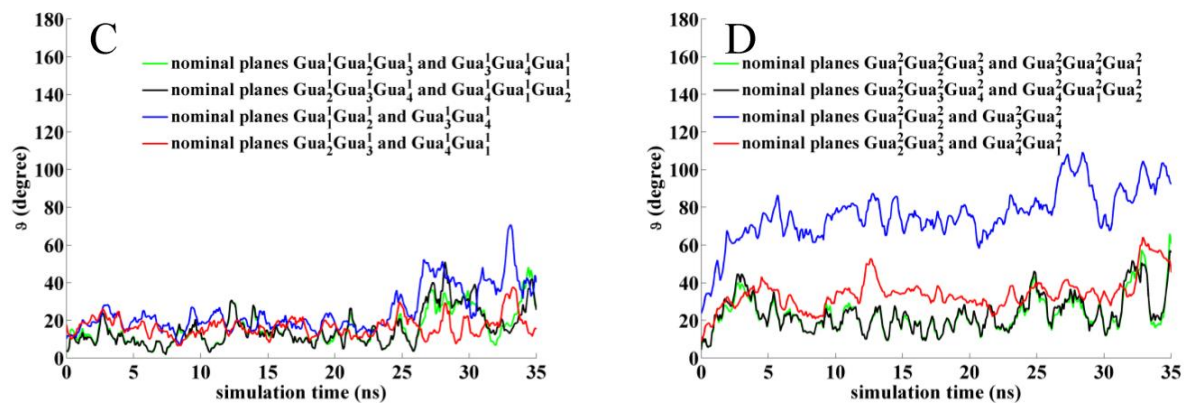


**Figure S6. Quartet planarity in the triazole-TBA GQ models 1 (A-D) and 2 (E-H).** A and E: Angles between the normals to the Gua planes in quartet 1 and axis Z (models 1 and 2, respectively; Z is a vector that joins the quartet 1 and 2 COMs; it does not strictly coincide with a normal to quartet 1); B and F: angles between the normal to the Gua planes in quartet 2 and axis Z (models 1 and 2, respectively); C and G: angles between the Gua planes in quartet 1 (models 1 and 2, respectively); D and H: angles between the Gua planes in quartet 2 (models 1 and 2, respectively).

## model 1



## model 2



**Figure S7. Quartet bending in triazole-TBA GQ.** A and C: “Lengthwise” and “diagonal” bending in quartet 1 (models 1 and 2, respectively). B and D: “Lengthwise” and “diagonal” bending in quartet 2 (models 1 and 2, respectively).