SUPPORTING MATERIAL

The systematic approach to describing conformational rearrangements in G-quadruplexes

Vladimir Tsvetkov*, Galina Pozmogova, Anna Varizhuk.*

*v.b.tsvetkov@gmail.com (V. Tsvetkov), annavarizhuk@gmail.com (A. Varizhuk)

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[a]	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+ ions (3-tetrad, monomolecular, parallel)	1 and 2 - similar	3.4	28
		2 and 3 - similar	3.4	29
352D[b]	d(TG_4T)[b] (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

[a] 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.
[b] Two distinct stacking arrangements are noted for GQ. COM distances and the twist angles in the table represent average values.

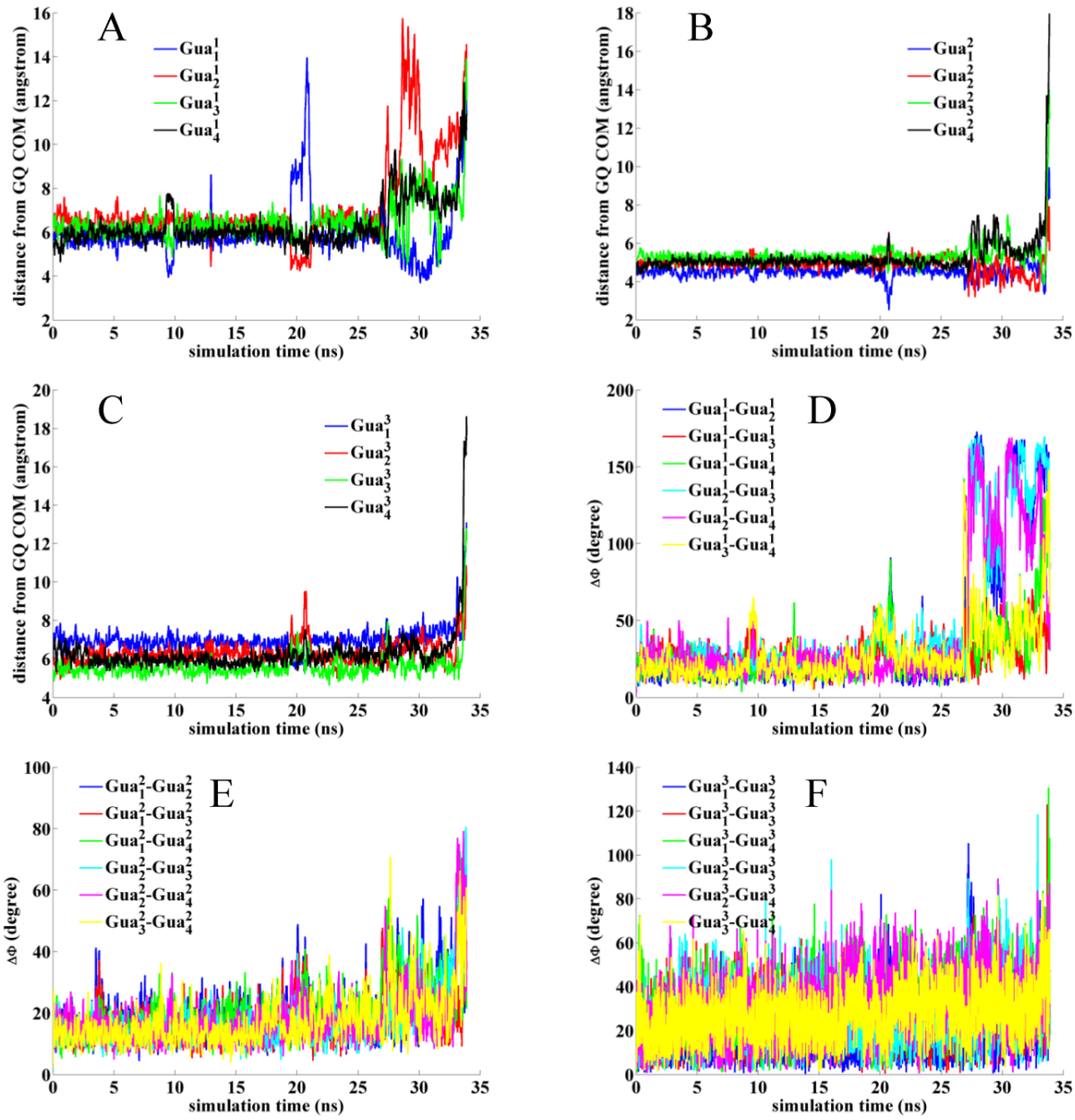


Figure S1. Quartet integrity (A-C) and planarity (D-F) in telGQ. A: Distances between the telGQ and Gua_1^1-Gua_4^1 COMs; B: distances between the telGQ and Gua_1^2-Gua_4^2 COMs; C: distances between the telGQ and Gua_1^3-Gua_4^3 COMs. D: Angles between the normals to the Gua planes in quartet 1; E: angles between the Gua planes in quartet 2; F: angles between the Gua planes in quartet 3.

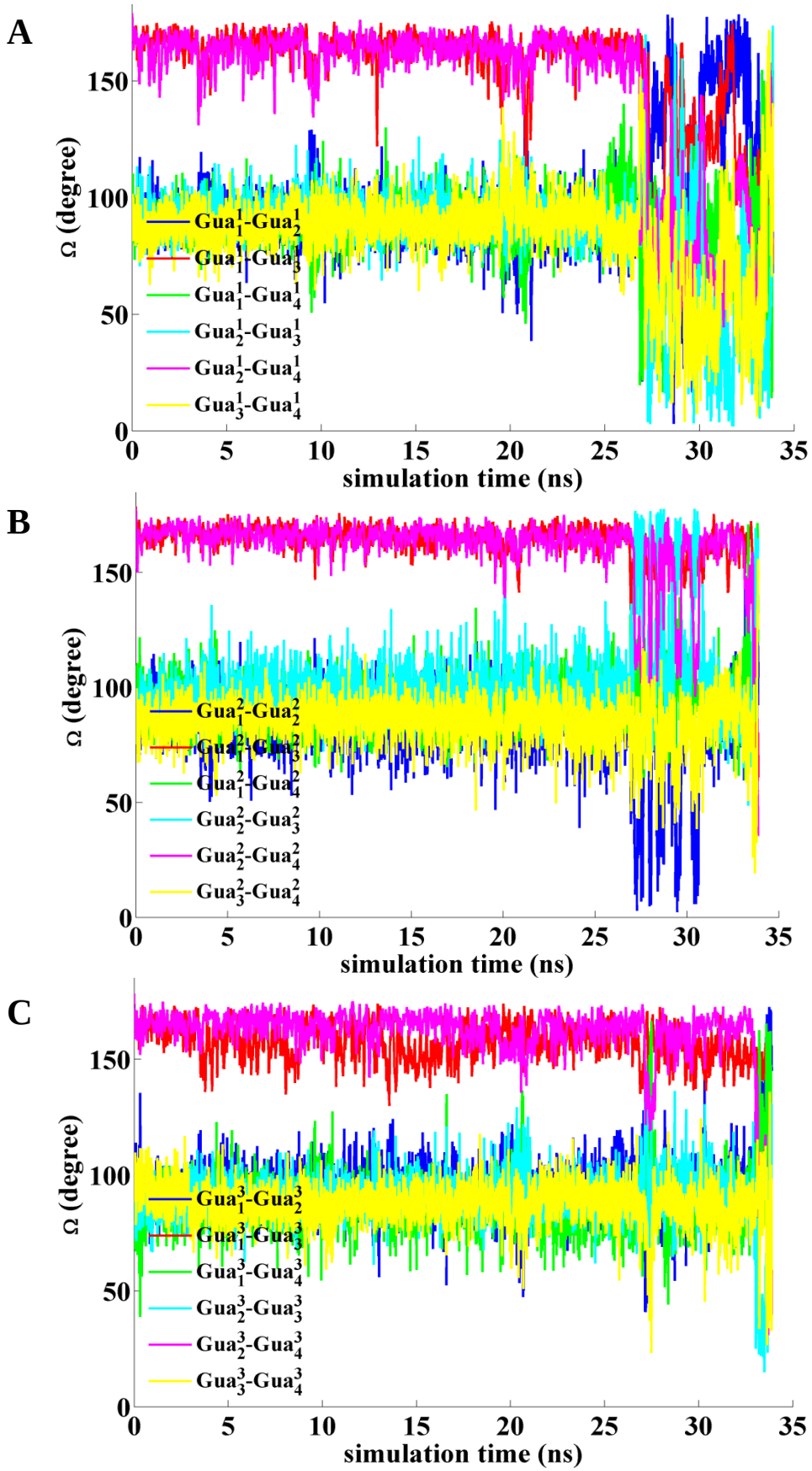
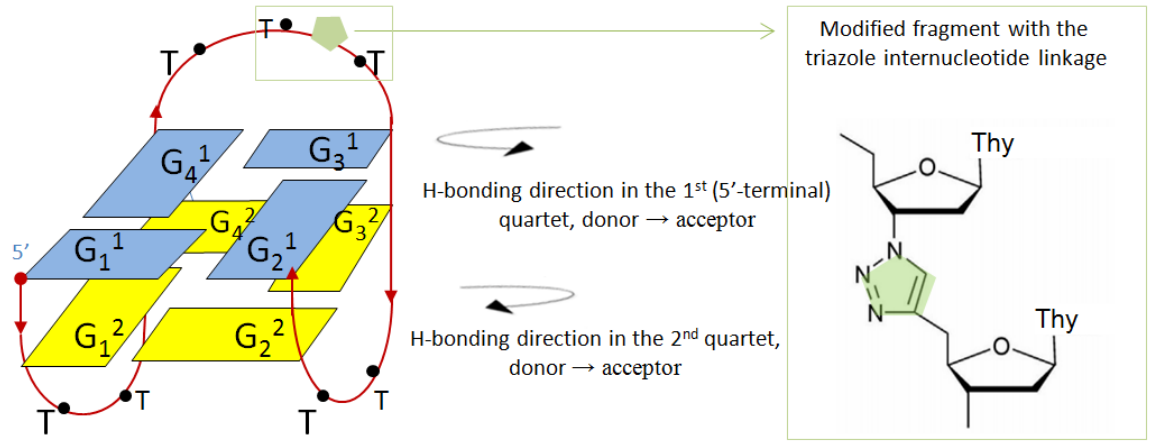


Figure S2. Relative Gua rotation in telGQ. A: Quartet 1; B: Quartet 2; C: Quartet 3.

Triazole-TBA – schematic representation



MD snapshots

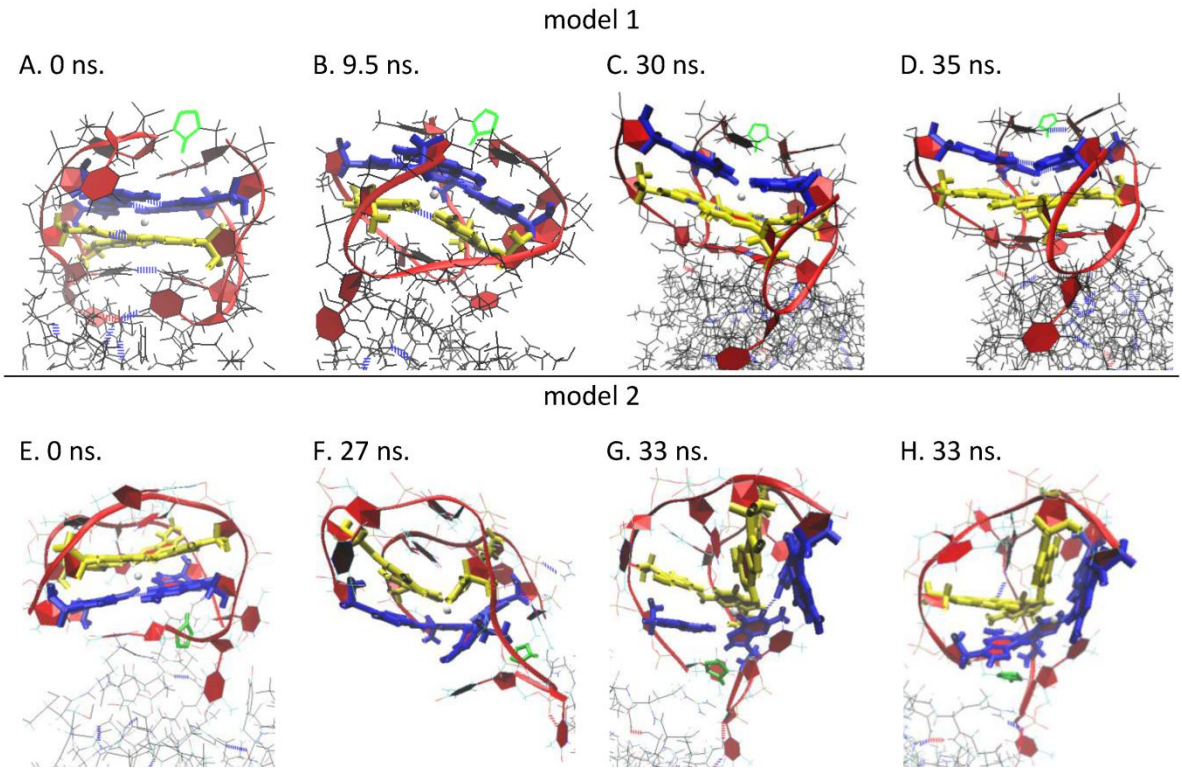


Figure S3. Triazole-TBA and MD simulation snapshots for its complex with thrombin. Quartet 1 is blue; quartet 2 is yellow. The triazole fragment in the modified internucleotide linkage is green. A: Model 1 at 0 ns. The quartets are intact and parallel. B: Model 1 at 9.5 ns. Insignificant "lateral" bending 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_2^1 and Gua_3^1 deviate from quartet 1. Gua_3^2 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.

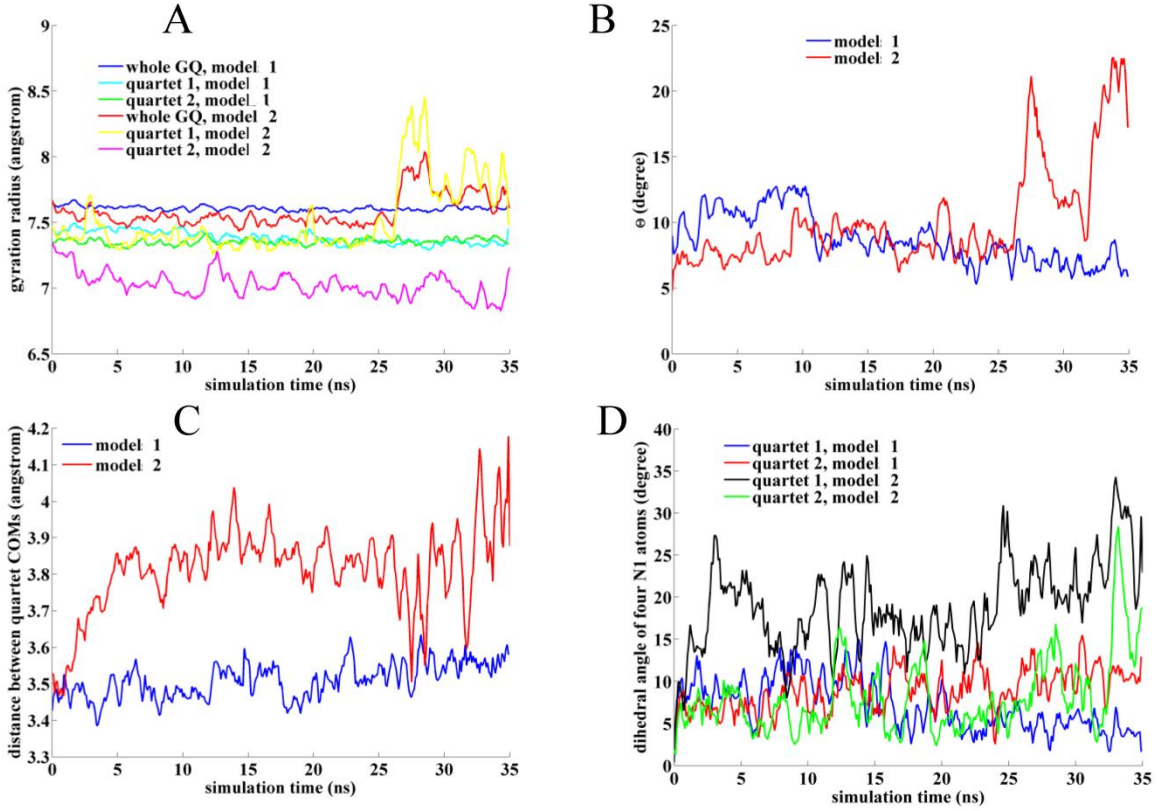


Figure S4. Basic GQ-related parameters and their fluctuations during triazole-TBA MD simulation. A: gyration radii; B: twist angles; C: distances between quartet COMs; D: the dihedral angles of the N1 atoms in each of the two quartets.

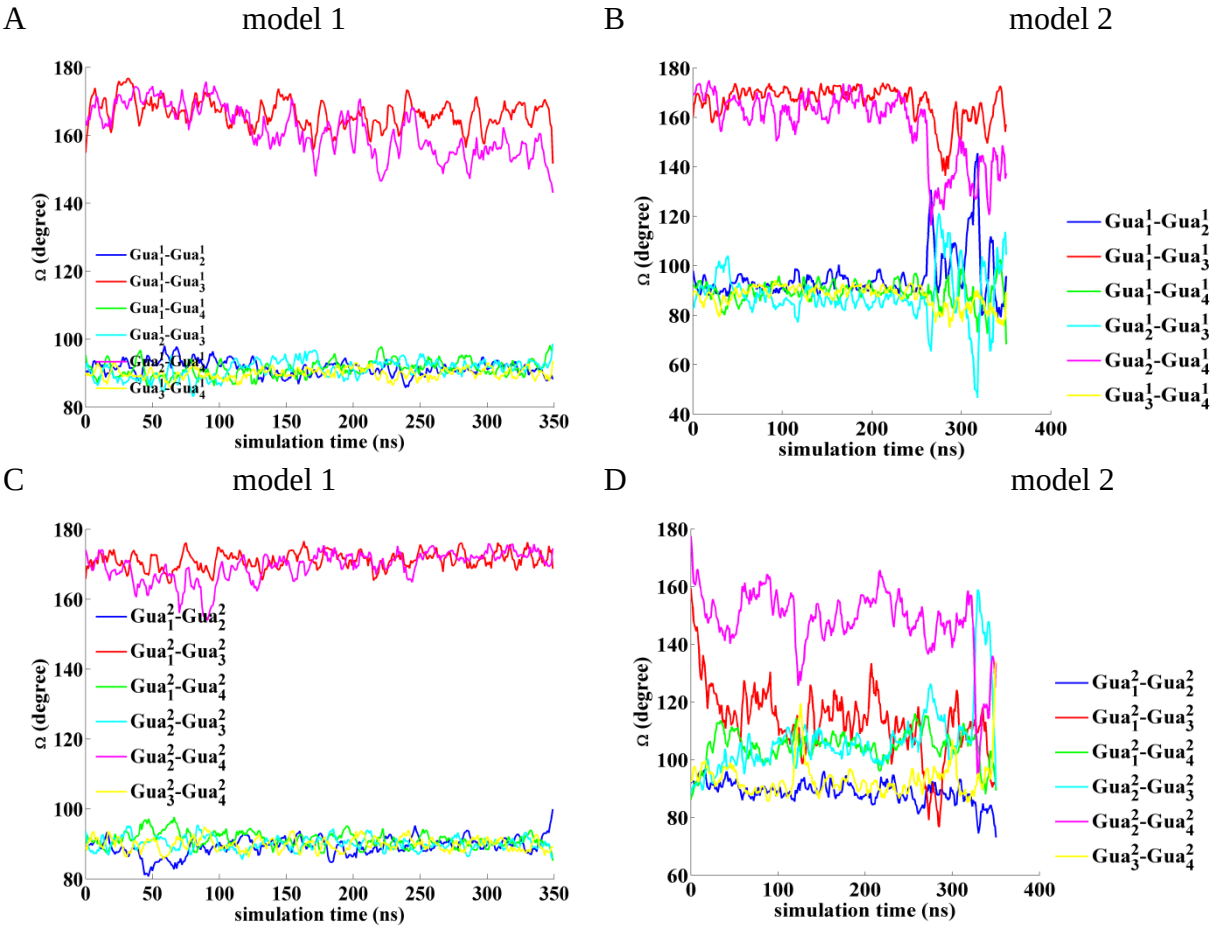


Figure S5. Relative Gua rotation in the triazole-TBA quartets 1 (A and C) and 2 (B and D)

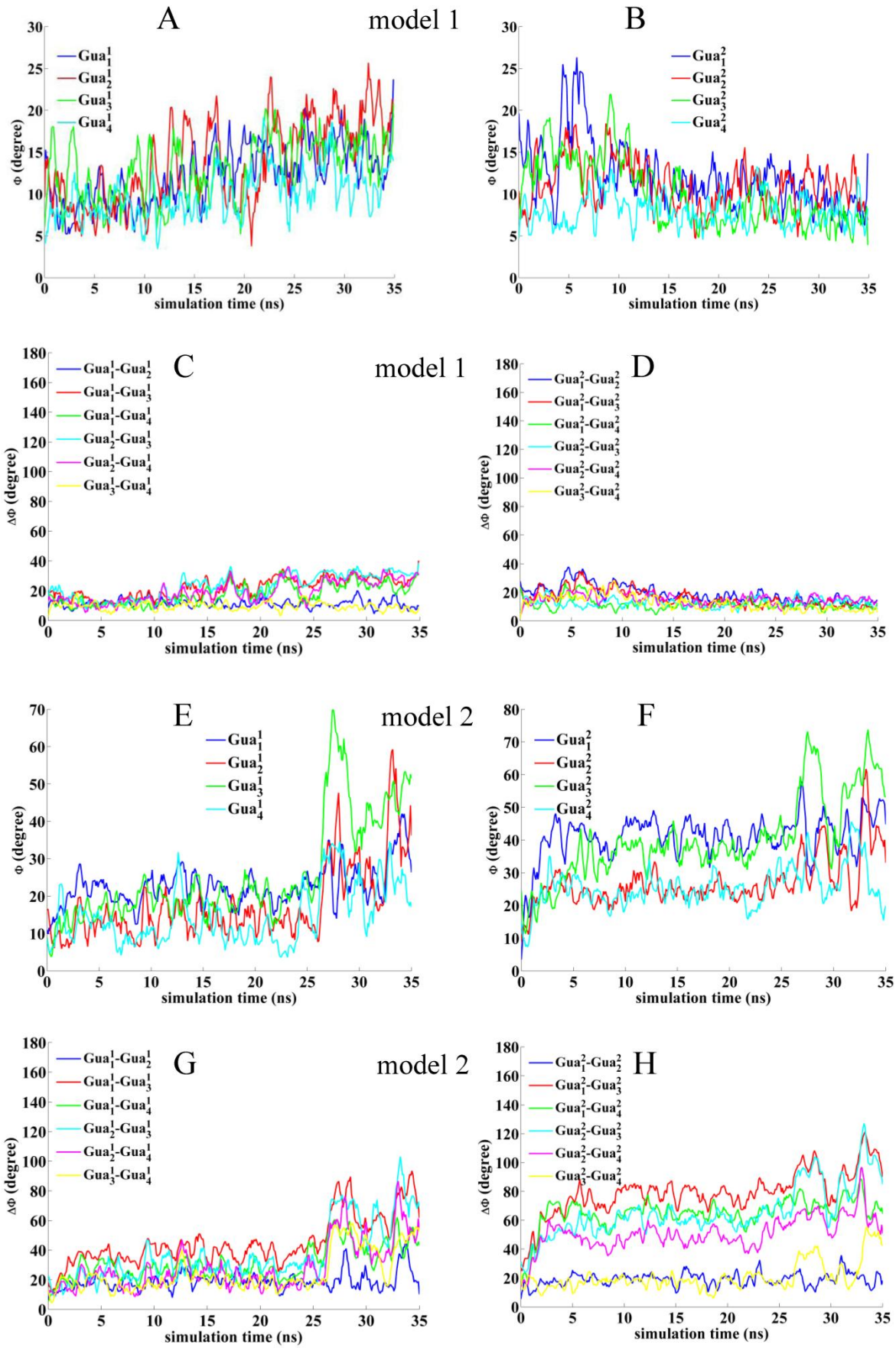


Figure S6. Quartet planarity in the triazole-TBA GQ models 1 (A-D) and 2 (E-H). A and E: Angles between the normals to the Gua planes in quartet 1 and axis Z (models 1 and 2, respectively; Z is a vector that joins the quartet 1 and 2 COMs; it does not strictly coincide with a normal to quartet 1); B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

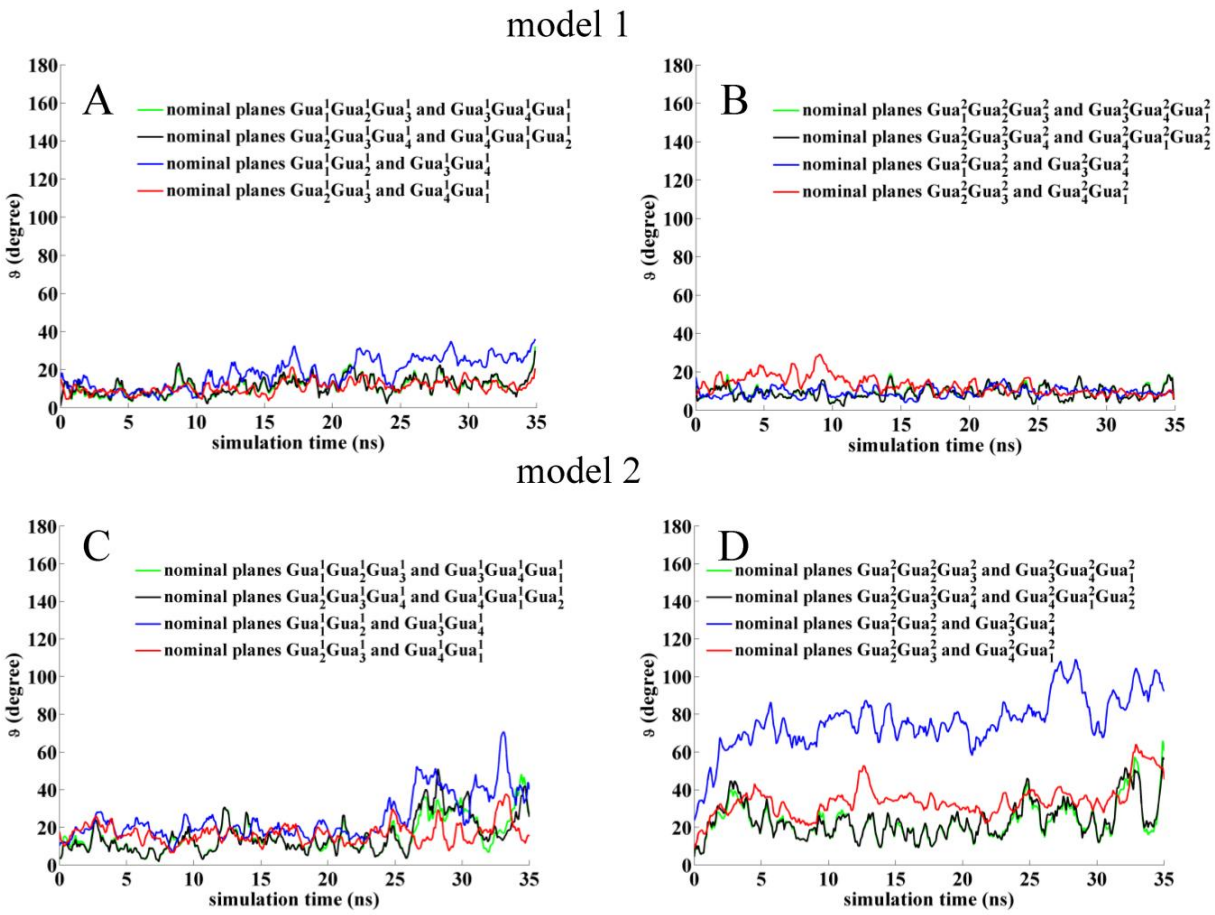


Figure S7. Quartet bending in triazole-TBA GQ. A and C: “Lengthwise” and “diagonal” bending in quartet 1 (models 1 and 2, respectively). B and D: “Lengthwise” and “diagonal” bending in quartet 2 (models 1 and 2, respectively).