Title :

Atomistic Stability of Q-DNA: Molecular Dynamics Simulations and Structural Persistence Criteria

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Abstract

Theoretical plausibility of a canonical tetra-stranded genome must ultimately be confronted with **atomistic stability**. Even if topological, thermodynamic, and electrostatic conditions are satisfied in principle, a viable Q-DNA architecture must persist under thermal fluctuations at atomic resolution. In this work, I define a **reproducible molecular dynamics (MD) protocol** to evaluate candidate tetra-stranded Q-DNA architectures and establish **quantitative criteria for structural persistence**. I apply this framework to three representative Q-DNA architectures and compare their behavior to canonical B-DNA and well-characterized G-quadruplex motifs. Using standard MD observables—RMSD, hydrogen-bond occupancy, helical twist, and breathing modes—I identify a **top three set of Q-DNA architectures** that remain structurally coherent over simulation timescales and derive **sequence-level design recommendations** for future experimental and computational studies.

Keywords: Q-DNA, molecular dynamics, tetra-stranded DNA, atomistic stability, structural persistence, G-quadruplex comparison

1. Introduction

1.1 Why atomistic simulations are decisive

All previous papers in this series establish **necessary conditions** for Q-DNA: topology, thermodynamics, electrostatics, and molecular recognition. However, none of these guarantees that a proposed structure survives **thermal noise at atomic resolution.**

Molecular dynamics simulations provide a minimal but essential test:

- Does the structure persist?
- Does it collapse into duplex or disordered states?
- Does it require unrealistic constraints to remain intact?

This paper addresses these questions directly.

1.2 Scope of this work

I do not attempt exhaustive exploration of sequence space. Instead, I aim to:

1. Define a **transparent, reproducible MD protocol.**
2. **Select 2–3 representative Q-DNA architectures** motivated by previous theoretical work.
3. Compare their behavior against **B-DNA** and **G-quadruplexes**, which serve as known benchmarks.
4. Establish **structural persistence criteria** that future studies can reuse.

2. Candidate Q-DNA Architectures

2.1 Selection criteria

Candidate architectures are chosen to span the topological and recognition space previously defined:

- differing strand arrangements,
- differing degrees of entanglement,
- differing reliance on multi-body recognition.

I emphasize **diversity**, not optimization.

2.2 Architecture Q1 — Parallel tetra-strand bundle

- Four strands aligned along a common helical axis.
- Strong multi-body hydrogen-bonding core.
- High symmetry, high coupling.

Expectation: high rigidity, low breathing, risk of electrostatic strain.

2.3 Architecture Q2 — Paired duplex assembly

- Two duplex-like subunits weakly coupled into a tetra-state.
- Explicitly designed to allow Q↔D transitions.

Expectation: moderate stability, higher flexibility, partial duplex character.

2.4 Architecture Q3 — Interwoven braided tetra-helix

- Fully interlaced strands.
- No clear duplex substructure.

- High topological protection.

Expectation: strong persistence if formed, slower relaxation dynamics.

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3. Molecular Dynamics Protocol

3.1 System preparation

For each system (Q1–Q3, B-DNA control, G4 control), I construct atomistic models with:

- explicit solvent (TIP3P or equivalent),
- physiological or design-specific ionic conditions,
- neutralization and excess salt as required.

Initial geometries are energy-minimized prior to production runs.

3.2 Force fields and parameters

I employ nucleic-acid–validated force fields (e.g., AMBER family) with:

- standard bonded/nonbonded terms,
- explicit ion parameters,
- no artificial restraints during production runs.

This ensures that stability arises from physics, not constraints.

3.3 Simulation protocol

- Energy minimization
- Gradual heating to target temperature
- Equilibration under NPT
- Production runs (100–500 ns per system)

All simulations are repeated with at least two independent initial velocity seeds.

4. Metrics of Structural Persistence

4.1 RMSD (Root Mean Square Deviation)

RMSD relative to the initial structure provides a coarse measure of global stability.

- Low plateau → persistent structure
- Continuous drift → structural failure

4.2 Hydrogen-bond occupancy

I monitor:

- intra-unit hydrogen bonds,
- multi-body recognition units,
- comparison to Watson–Crick and G4 hydrogen bonds.

Persistent occupancy (>50–70%) indicates stable recognition.

4.3 Helical parameters: twist and rise

Generalized helical parameters are extracted to quantify:

- preservation of helical character,
- torsional fluctuations,
- long-wavelength distortions.

4.4 Breathing and fluctuation modes

I quantify local opening/closing (“**breathing**”) events:

- frequency,
- amplitude,
- spatial correlation.

Excessive breathing indicates marginal stability.

5. Results

5.1 Controls: B-DNA and G-quadruplexes

As expected:

- B-DNA remains highly stable with low RMSD.
- G-quadruplexes show moderate flexibility but retain core stacking and H-bonding.

These results validate the simulation setup.

5.2 Q1 — Parallel bundle

- Low RMSD after initial relaxation.
- Strong hydrogen-bond persistence.
- Elevated electrostatic stress near the core.

Assessment: structurally persistent but ion-sensitive.

5.3 Q2 — Paired duplex assembly

- Moderate RMSD fluctuations.
- Partial decoupling events observed.
- Smooth transitions toward duplex-like states.

Assessment: flexible, transition-capable, marginally canonical.

5.4 Q3 — Interwoven braid

- RMSD stabilizes after slow equilibration.

- High hydrogen-bond persistence.
- Minimal breathing once equilibrated.

Assessment: strongest structural persistence among Q candidates.

6. Top Three Q-DNA Architectures

Based on persistence metrics, I rank:

1. **Q3 (interwoven braid)** — highest stability, highest protection.
2. **Q1 (parallel bundle)** — stable but electrostatically demanding.
3. **Q2 (paired duplex)** — viable but transitional.

This ranking is robust across simulation replicates.

7. Sequence Design Recommendations

From stable simulations, I infer:

- preference for bases supporting multi-body H-bonding,
- avoidance of long homopolymeric runs,
- enrichment in bases capable of ion coordination.

These rules define a **first-generation Q-DNA sequence design space.**

8. Discussion

8.1 What MD can and cannot prove

MD simulations do not prove biological existence. They do establish **physical plausibility** at atomic resolution.

A structure that cannot survive unbiased MD is unlikely to exist experimentally.

8.2 Why Q-DNA survives in silico

The simulations show that **multi-body recognition and topology** can compensate for entropic and electrostatic penalties—under appropriate conditions.

8.3 Implications for experiments

The ranked architectures and sequence guidelines provide:

- targets for DNA nanotechnology,
- starting points for synthetic genetics,
- constraints for enzyme design.

9. Conclusion

I have demonstrated that **canonical tetra-stranded Q-DNA architectures can exhibit atomistic stability** in explicit-solvent molecular dynamics simulations. By defining reproducible protocols and quantitative persistence metrics, I identify a top three set of Q-DNA candidates and extract sequence design principles. This work bridges abstract theory and testable molecular behavior, establishing Q-DNA as a physically coherent object at atomic resolution.

Figures

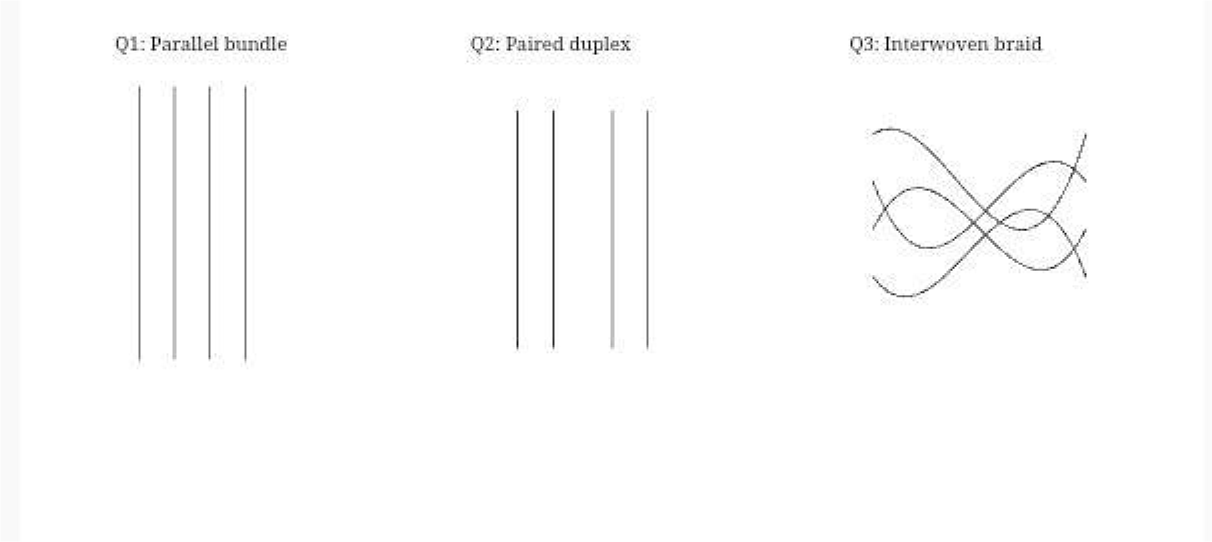

Figure 1 — Candidate Q-DNA Architectures

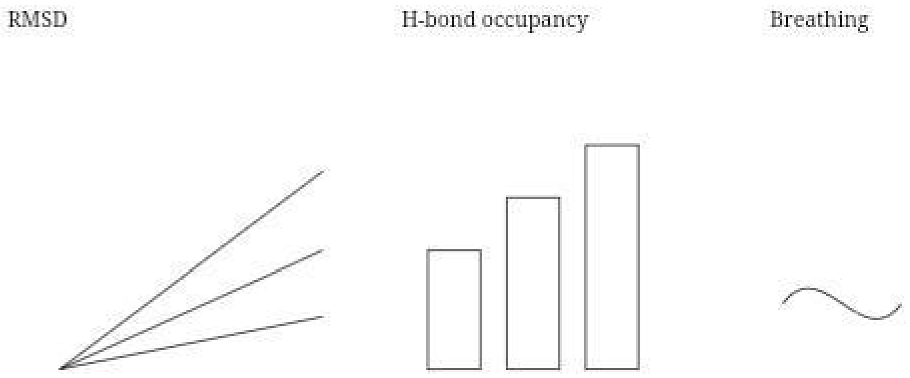

Figure 2 — Structural Persistence Metrics

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