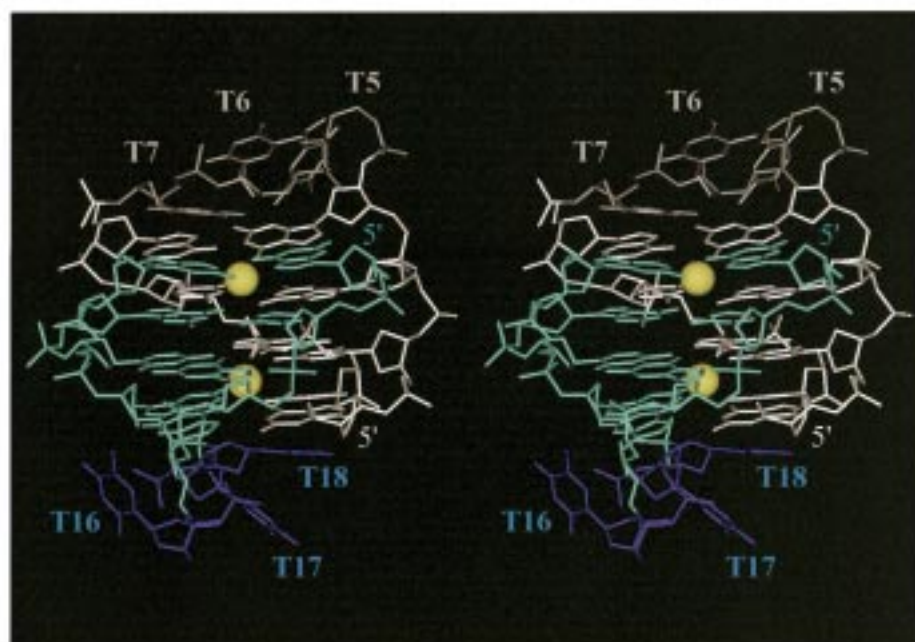Stereo representation of starting coordinates and theoretical structures

Supplementary material to Spackova, N; Berger, I.; Sponer, J.
*Structural dynamics and cation interactions of DNA quadruplex molecules
containing mixed guanine/cytosine quartets revealed by large-scale MD simulations*

d(GCGGTTTGCGG)2; NaCl, NMR structure (Ref. 9a)

Chains are in blue and white, corresp. thymine loops
are colored dark blue and gray, respectively.
Sodium ions are shown as larger spheres in yellow.
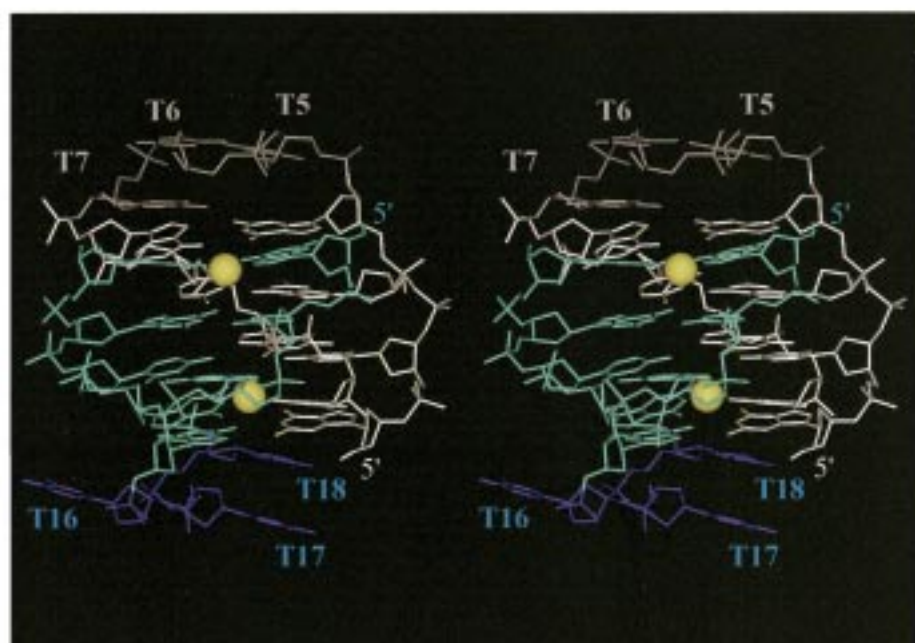
Simulation A7L (see Table I)
Averaged structure 1.5-2.5ns,
color coding as above.

Spackova N.; Berger, I.; Sponer, J. *"Structural dynamics and cation interactions..."*   I.
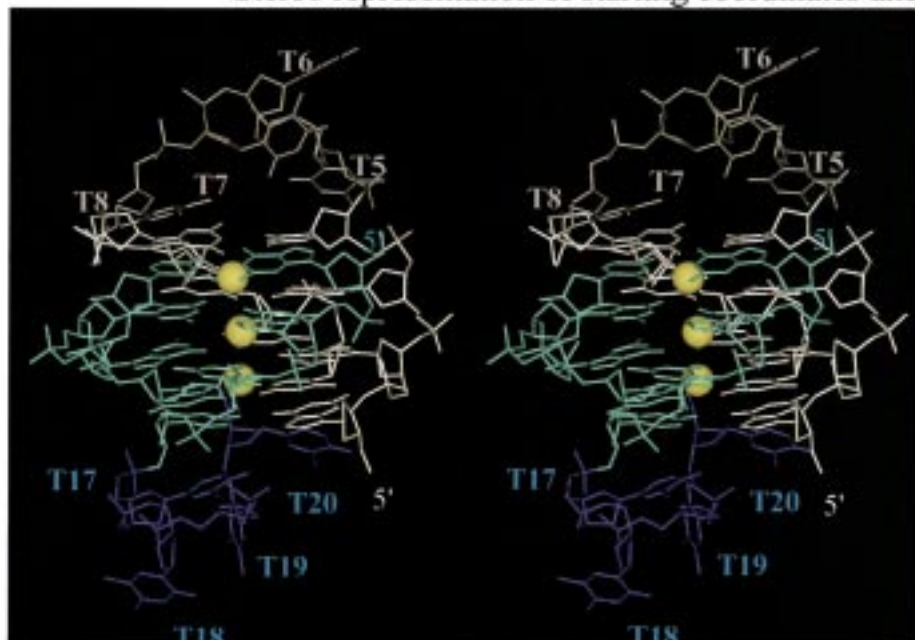
d(GGGCTTTTGGGC)2; NaCl, NMR structure (Ref. 9b)

Chains are in blue and white, corresp. thymine loops are colored dark blue and gray, respectively. Sodium ions are shown as larger spheres in yellow.
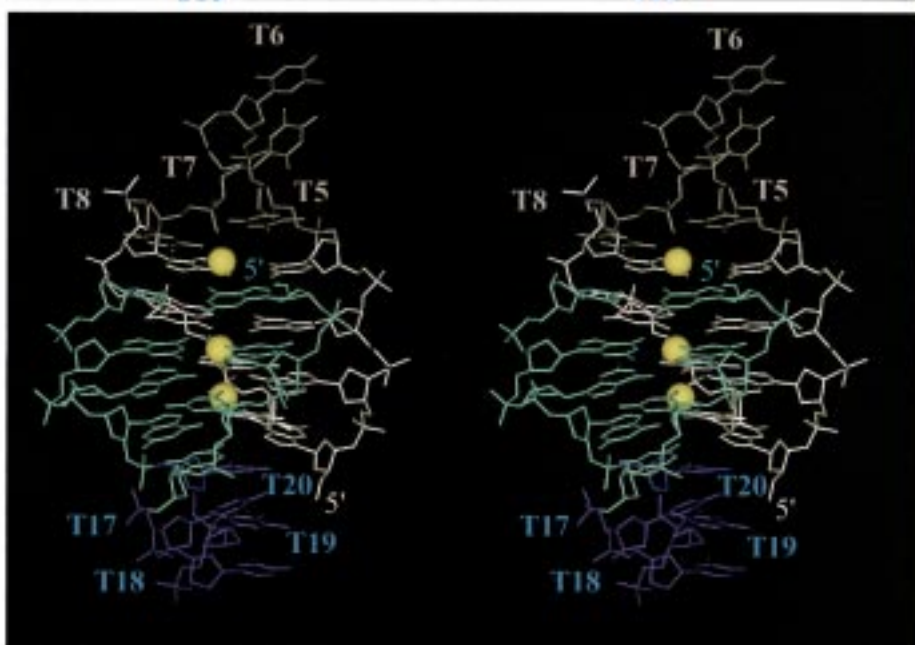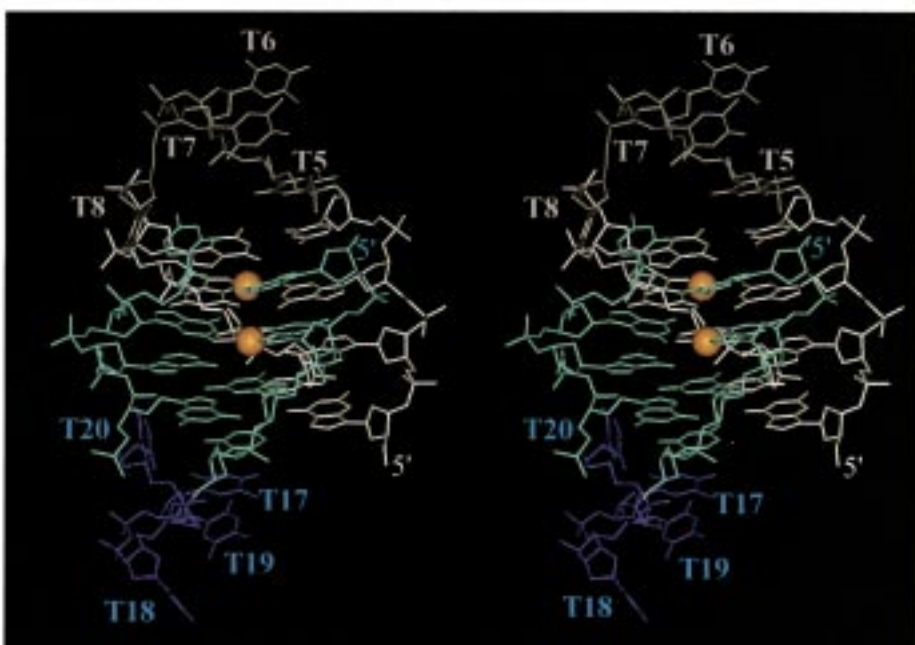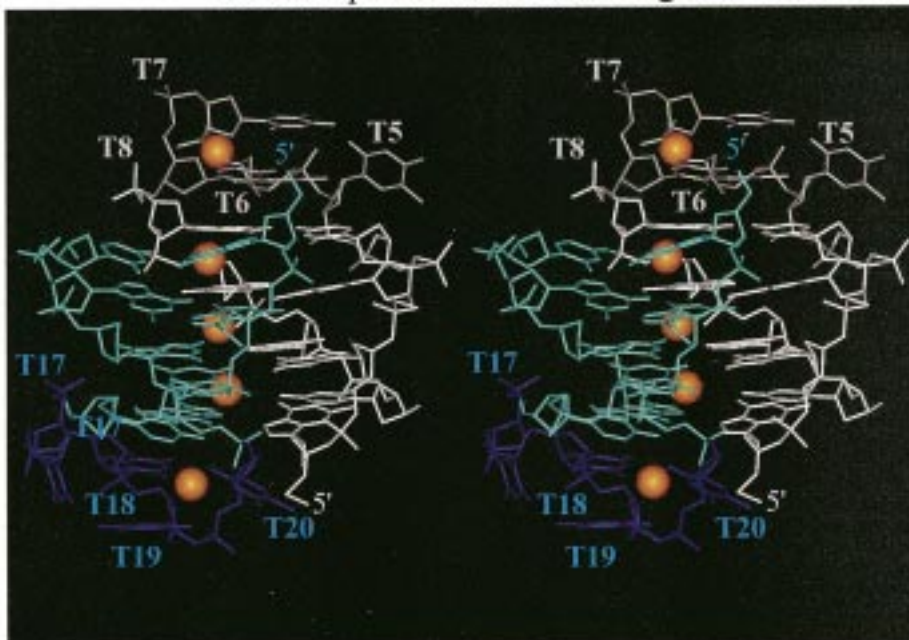
Note T6 and T18 residues projecting away from the molecule (see text).

Simulation B5L (see Table I). Average structure 4-5ns, color coding as above.
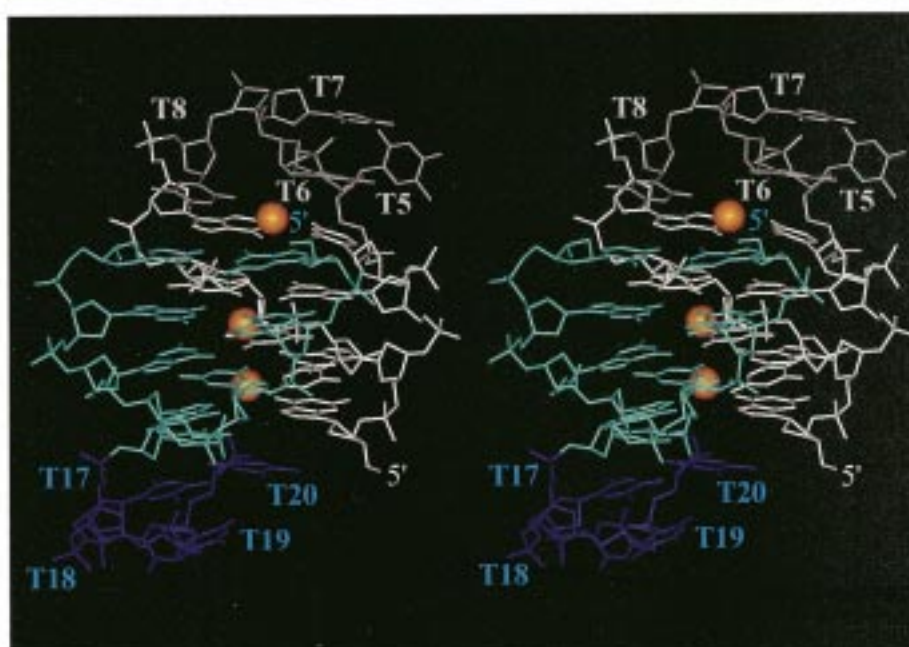
Simulation B6L (see Table I). Average structure 4-5ns. Color coding as above, except potassium ions that are drawn as larger spheres in orange.
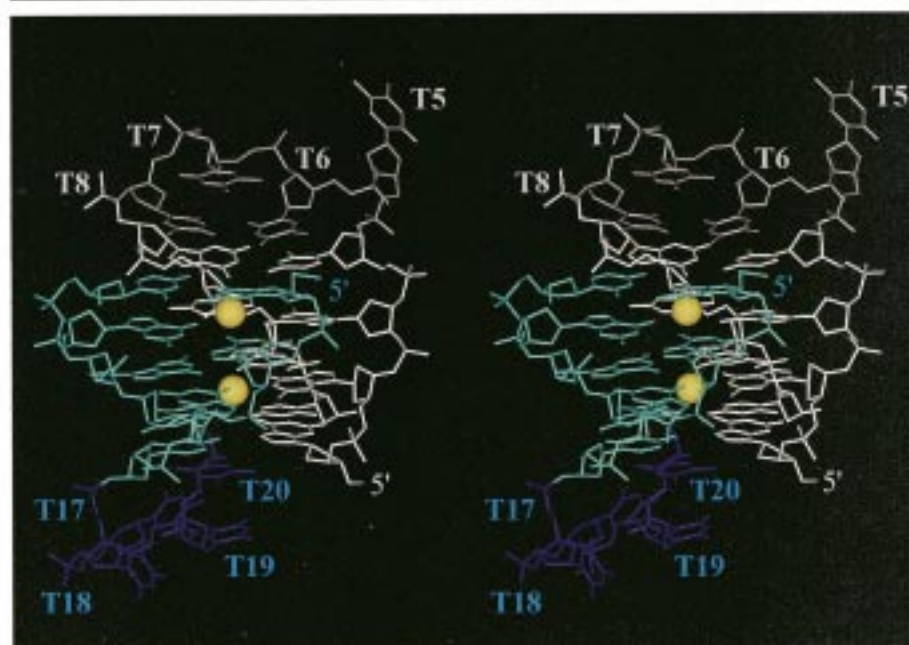
Spackova N.; Berger, I.; Sponer, J. *"Structural dynamics and cation interactions..."*   II.

Stereo representation of starting coordinates and theoretical structures

d(GGGCTTTTGGGC)2; KCl, NMR structure (Ref. 9c)

Chains are in blue and white, corresp. thymine loops are colored dark blue and gray, respectively. Potassium ions are shown as larger spheres in orange.
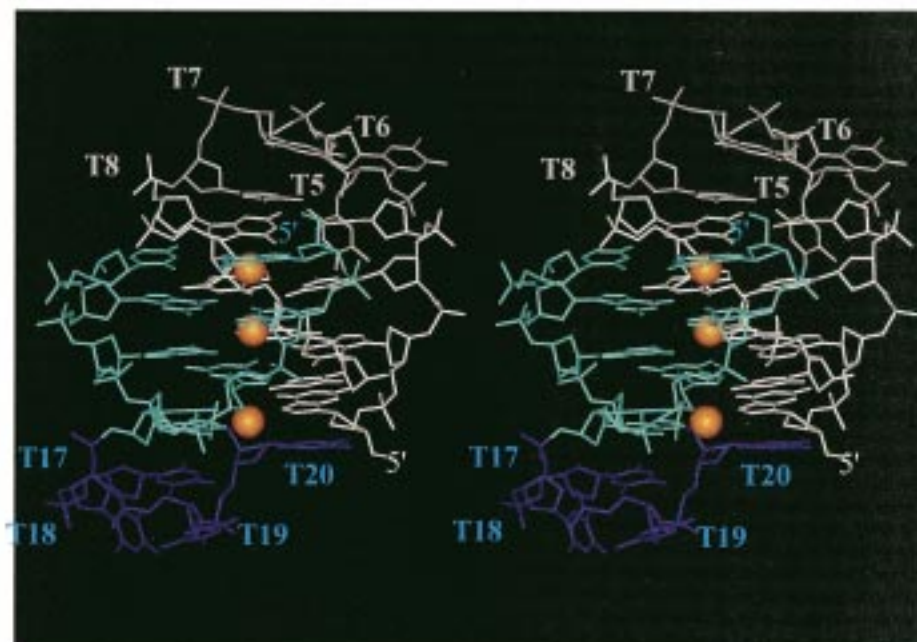
Simulation B3L (see Table I) Averaged structure 3.9-4.9ns, color coding as above.

Simulation B4L (see Table I) Averaged structure 3-4ns. Color coding as above, except for sodium ions that are shown as larger spheres in yellow.

Spackova N.; Berger, I.; Sponer, J. *"Structural dynamics and cation interactions..."*   IIIa.

Stereo representation of starting coordinates and theoretical structures

d(GGGCTTTTGGGC)2; KCl, NMR starting structure (Ref. 9c)

Simulation B7L (see Table I)
Averaged structure 11-12ns,
color coding as before.
Modified Cornell *et al*. force field.
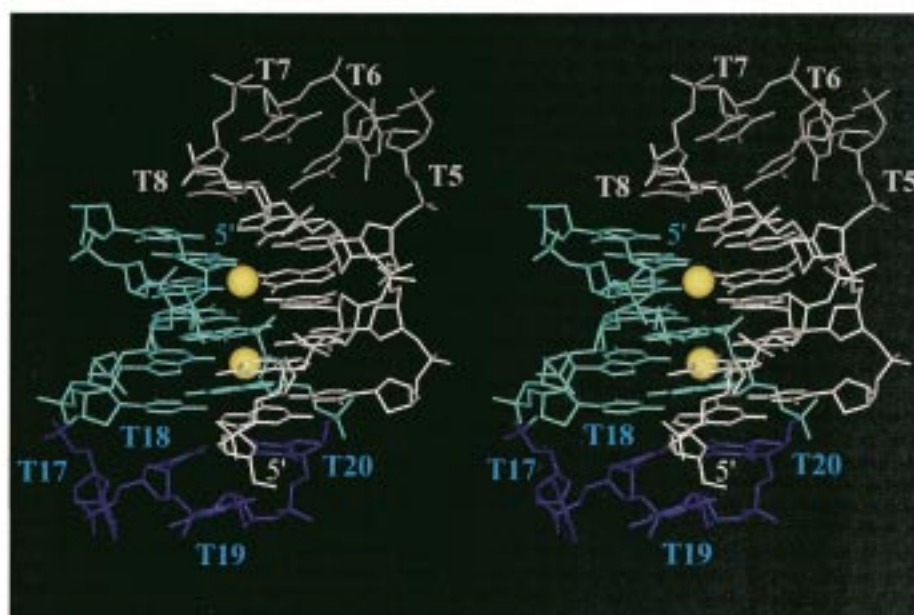
Simulation B8L (see Table I)
Averaged structure 9-10ns,
color coding as above except for
sodium ions drawn in yellow.
Force field as above.

Spackova N.; Berger, I.; Sponer, J. "*Structural dynamics and cation interactions...*"

IIIb.

Stereo representation of starting coordinates and theoretical structures

d(GGGCTTTTGGGC)₂; KCl, NMR starting structure (Ref. 9c)

Simulation B9L (see Table I)
Averaged structure 4-5ns, color coding as before.
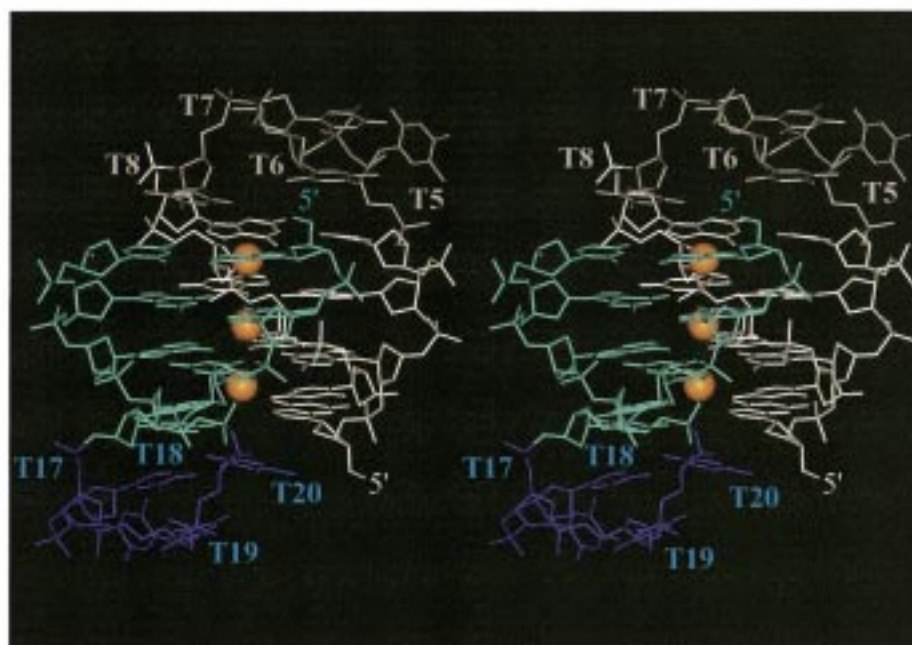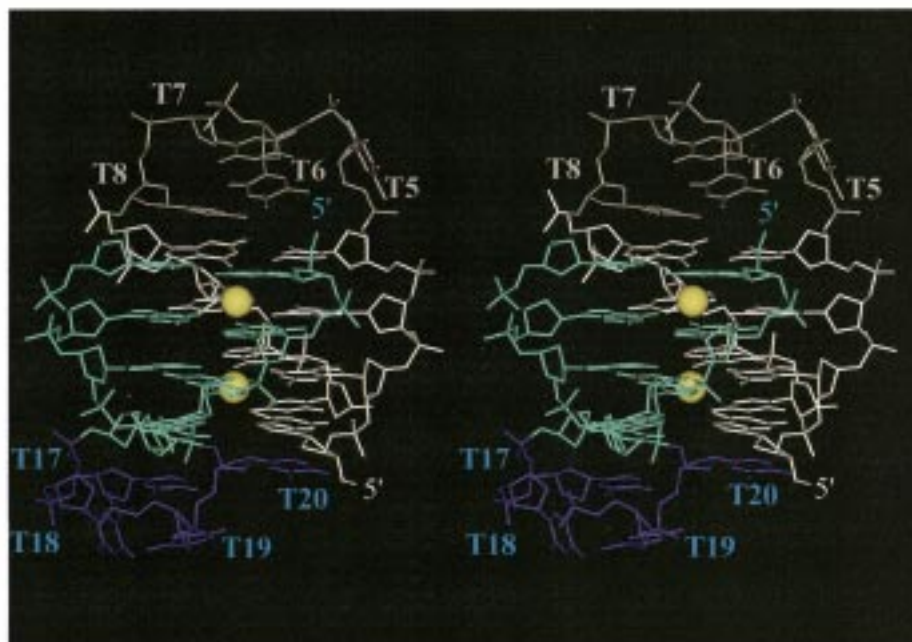Same as B7L; with modified equilibration protocol
and modified Cornell *et al.* force field.

Simulation B11L (see Table I)
Averaged structure 4-5ns,
color coding as above except for
sodium ions drawn in yellow.
High salt simulation.

Spackova N.; Berger, I.; Sponer, J. *"Structural dynamics and cation interactions..."*   IIIc.

Stereo representation of starting coordinates and theoretical structures

d(GGGCTTTTGGGC)2; KCl, NMR starting structure (Ref. 9c)
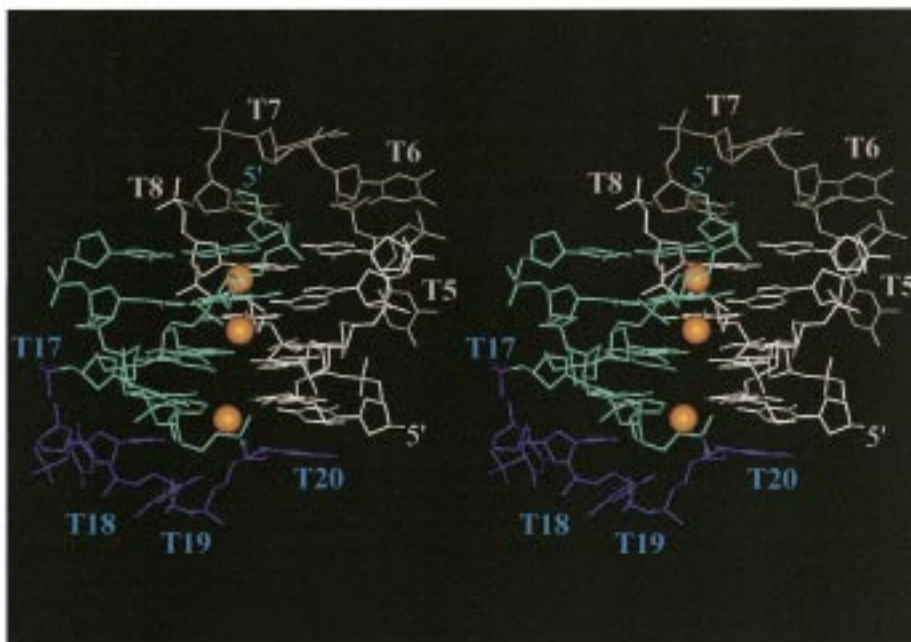
Snapshot from simulation B7L at 10ns,
starting geometry for simulation B10L (below).
Color coding as before.
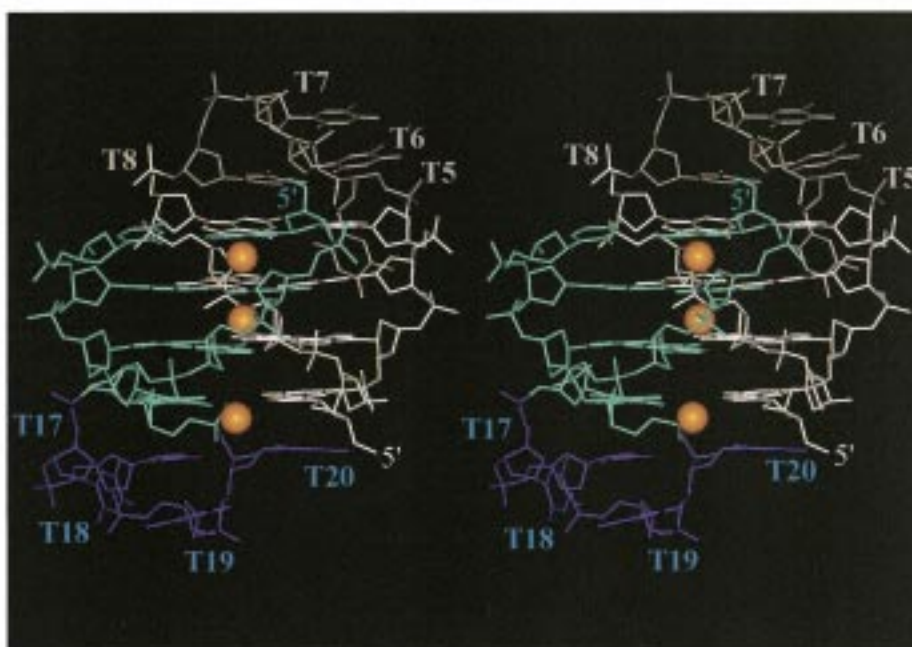
Simulation B10L (see Table I)
Averaged structure 2.5-3ns.
Modified Cornell *et al.* force field.

Spackova N.; Berger, I.; Sponer, J. *"Structural dynamics and cation interactions..."*   IIId.

Stereo representation of representative loop geometries
and ion-loop interactions in simulated structures based on
d(GGGCTTTTGGGC)2 NMR starting coordinates (Ref. 9c)

Ion - loop interaction A
Residues are colored by atom type,
Sodium is drawn as a larger
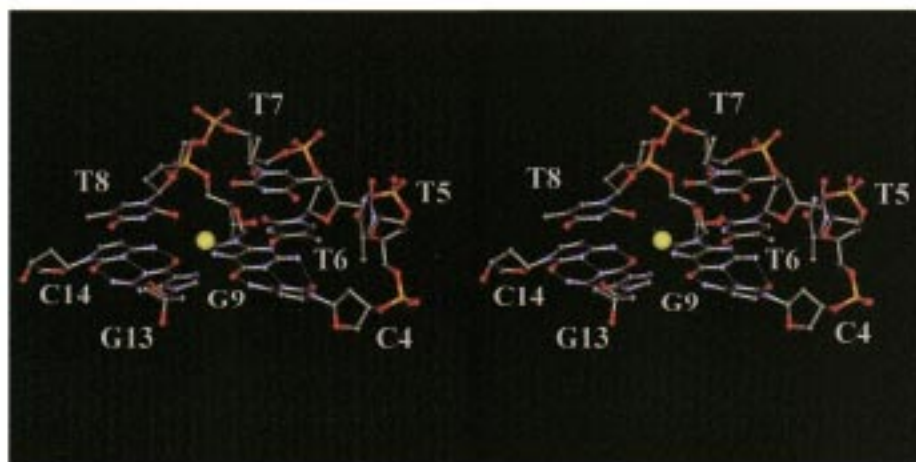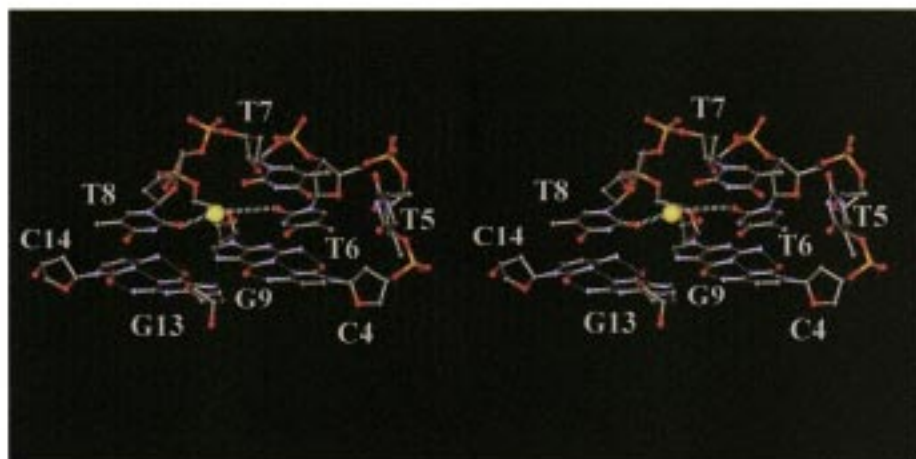sphere in yellow.

The ion resides above the mixed
GCGC quartet layer that adopts a
sheared conformation.
Note stacked thymines T6 and T7.
Dashed lines indicate hydrogen bond
interactions..

Ion - loop interaction B
Color coding as above.

The ion is coordinated to residues
thymines T6 and T8, interacting with
O2 keto oxygen atoms (thick dashed
lines).
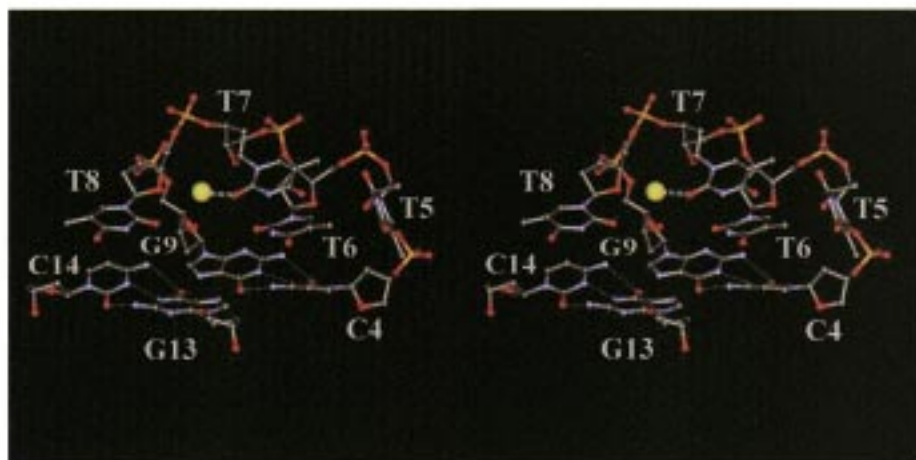
Ion - loop interaction C
Color coding as above.

The ion resides at the loop apex,
interacting with the O2 keto oxygen
of residue thymine T7.

Spackova N.; Berger, I.; Sponer, J. *"Structural dynamics and cation interactions..."*   IV.

Supplementary material – PDB files

Coordinate files in PDB format for all initial structures utilized in simulations with thymidine loops and for all final structures with thymidine loops. PDB files were submitted via electronic mail to pdb.ja@acs.org.
Coordinates are not presented in this printed material.

Headers of presented PDB files:

```
REMARK  description: initial structure 1A6H (PDB database), ref.9a
REMARK  NMR structure
REMARK  sequence: d(GCGGTTTGCGG)2
REMARK  number of integral cations inside the solute: two
REMARK  PDB format: output from the Carnal module of AMBER5.0


REMARK  description: initial structure 1A8N (PDB database), ref.9b
REMARK  NMR structure obtained in presence of NaCl
REMARK  sequence: d(GGGCTTTTGGGC)2
REMARK  number of integral cations inside the solute: three
REMARK  PDB format: output from the Carnal module of AMBER5.0


REMARK  description: initial structure 1A8W (PDB database), ref.9c
REMARK  NMR structure obtained in presence of KCl
REMARK  sequence: d(GGGCTTTTGGGC)2
REMARK  number of integral cations inside the solute: five
REMARK  PDB format: output from the Carnal module of AMBER5.0


REMARK  description: snapshot from simulation B7L at 10 ns (see Table 1)
REMARK  initial structure for simulation B10L
REMARK  sequence: d(GGGCTTTTGGGC)2
REMARK  number of integral cations inside the solute: three
REMARK  PDB format: output from the Carnal module of AMBER5.0


REMARK  name: A7L (see Table 1)
REMARK  description: averaged structure from the interval 1.5-2.5 ns
REMARK  simulation carried out in presence of Na+
REMARK  sequence: d(GCGGTTTGCGG)2
REMARK  initial structure: 1A6H (PDB database), two internal cations
REMARK  number of integral cations inside the solute at the end
REMARK  of simulation: two
REMARK  PDB format: output from the Carnal module of AMBER5.0


REMARK  name: B3L (see Table 1)
REMARK  description: averaged structure from the interval 3.9-4.9 ns
REMARK  simulation carried out in presence of K+
REMARK  sequence: d(GGGCTTTTGGGC)2
REMARK  initial structure: 1A8W (PDB database), five internal cations
REMARK  number of integral cations inside the solute at the end
REMARK  of simulation: three
REMARK  PDB format: output from the Carnal module of AMBER5.0
```

```
REMARK  name: B4L (see Table 1)
REMARK  description: averaged structure from the interval 3-4 ns
REMARK  simulation carried out in presence of Na+
REMARK  sequence: d(GGGCTTTTGGGC)2
REMARK  initial structure: 1A8W (PDB database), five internal cations
REMARK  number of integral cations inside the solute at the end
REMARK  of simulation: two
REMARK  PDB format: output from the Carnal module of AMBER5.0


REMARK  name: B5L (see Table 1)
REMARK  description: averaged structure from the interval 4-5 ns
REMARK  simulation carried out in presence of Na+
REMARK  sequence: d(GGGCTTTTGGGC)2
REMARK  initial structure: 1A8N (PDB database), three internal cations
REMARK  number of integral cations inside the solute at the end
REMARK  of simulation: three
REMARK  PDB format: output from the Carnal module of AMBER5.0


REMARK  name: B6L (see Table 1)
REMARK  description: averaged structure from the interval 4-5 ns
REMARK  simulation carried out in presence of K+
REMARK  sequence: d(GGGCTTTTGGGC)2
REMARK  initial structure: 1A8N (PDB database), three internal cations
REMARK  number of integral cations inside the solute at the end
REMARK  of simulation: two
REMARK  PDB format: output from the Carnal module of AMBER5.0


REMARK  name: B7L (see Table 1)
REMARK  description: averaged structure from the interval 11-12 ns
REMARK  simulation carried out in presence of K+
REMARK  sequence: d(GGGCTTTTGGGC)2
REMARK  initial structure: 1A8W (PDB database), five internal cations
REMARK  number of integral cations inside the solute at the end
REMARK  of simulation: three
REMARK  PDB format: output from the Carnal module of AMBER5.0


REMARK  name: B8L (see Table 1)
REMARK  description: averaged structure from the interval 9-10 ns
REMARK  simulation carried out in presence of Na+
REMARK  sequence: d(GGGCTTTTGGGC)2
REMARK  initial structure: 1A8W (PDB database), five internal cations
REMARK  number of integral cations inside the solute at the end
REMARK  of simulation: two
REMARK  PDB format: output from the Carnal module of AMBER5.0


REMARK  name: B9L (see Table 1)
REMARK  description: averaged structure from the interval 4-5 ns
REMARK  simulation carried out in presence of K+
REMARK  sequence: d(GGGCTTTTGGGC)2
REMARK  initial structure: 1A8W (PDB database), five internal cations
REMARK  number of integral cations inside the solute at the end
REMARK  of simulation: three
REMARK  PDB format: output from the Carnal module of AMBER5.0
```

```
REMARK   name: B10L (see Table 1)
REMARK   description: averaged structure from the interval 2.5-3.0 ns
REMARK   simulation carried out in presence of K+
REMARK   sequence: d(GGGCTTTTGGGC)2
REMARK   initial structure: snapshot from simulation B7L at 10 ns
REMARK   number of integral cations inside the solute at the end
REMARK   of simulation: three
REMARK   PDB format: output from the Carnal module of AMBER5.0


REMARK   name: B11L (see Table 1)
REMARK   description: averaged structure from the interval 4-5 ns
REMARK   simulation carried out in presence of Na+ (high salt concentration)
REMARK   sequence: d(GGGCTTTTGGGC)2
REMARK   initial structure: 1A8W (PDB database), five internal cations
REMARK   number of integral cations inside the solute at the end
REMARK   of simulation: two
REMARK   PDB format: output from the Carnal module of AMBER5.0
```