

Figure S1. The aromatic to H1' region of the 250 ms NOESY spectrum of tc-DNA•DNA hybrid. The sequential H8/6-H1' connectivity pathways are indicated with green lines for the tc-DNA strand and yellow for the DNA strand.

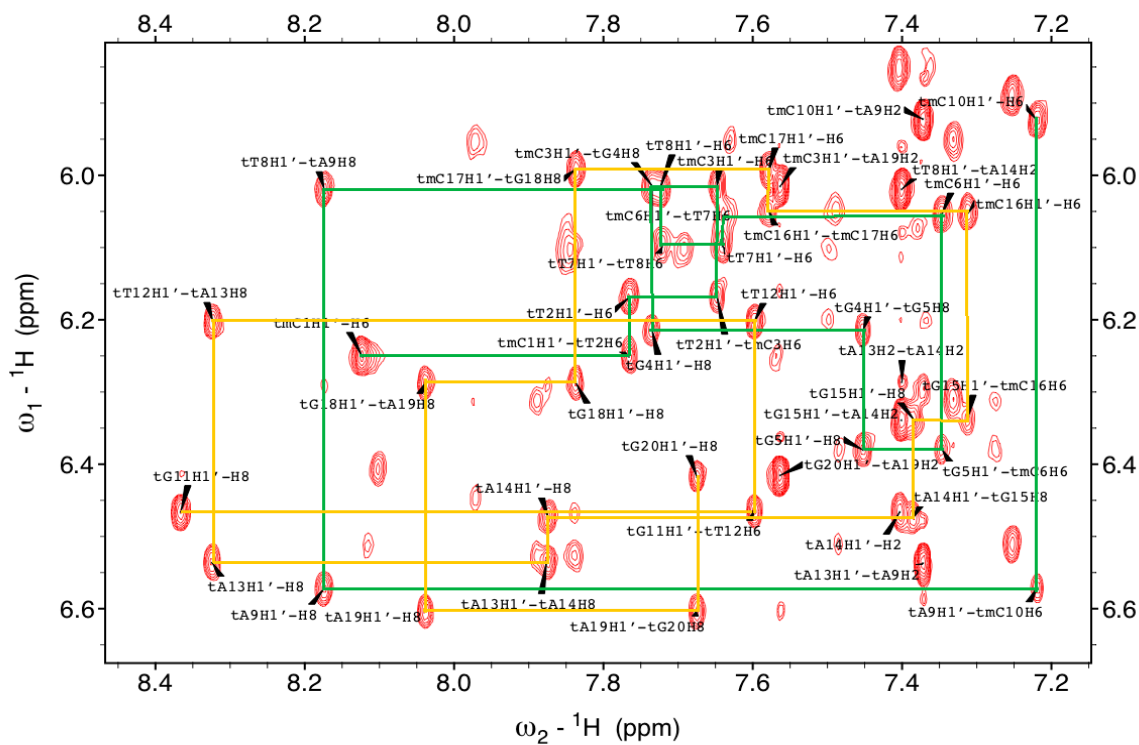


Figure S2. The aromatic to H1' region of the 250 ms NOESY spectrum of tc-DNA•tc-DNA duplex. The sequential H8/6-H1' connectivity pathways are indicated with green lines for the first tc-DNA strand and yellow for the second tc-DNA strand.

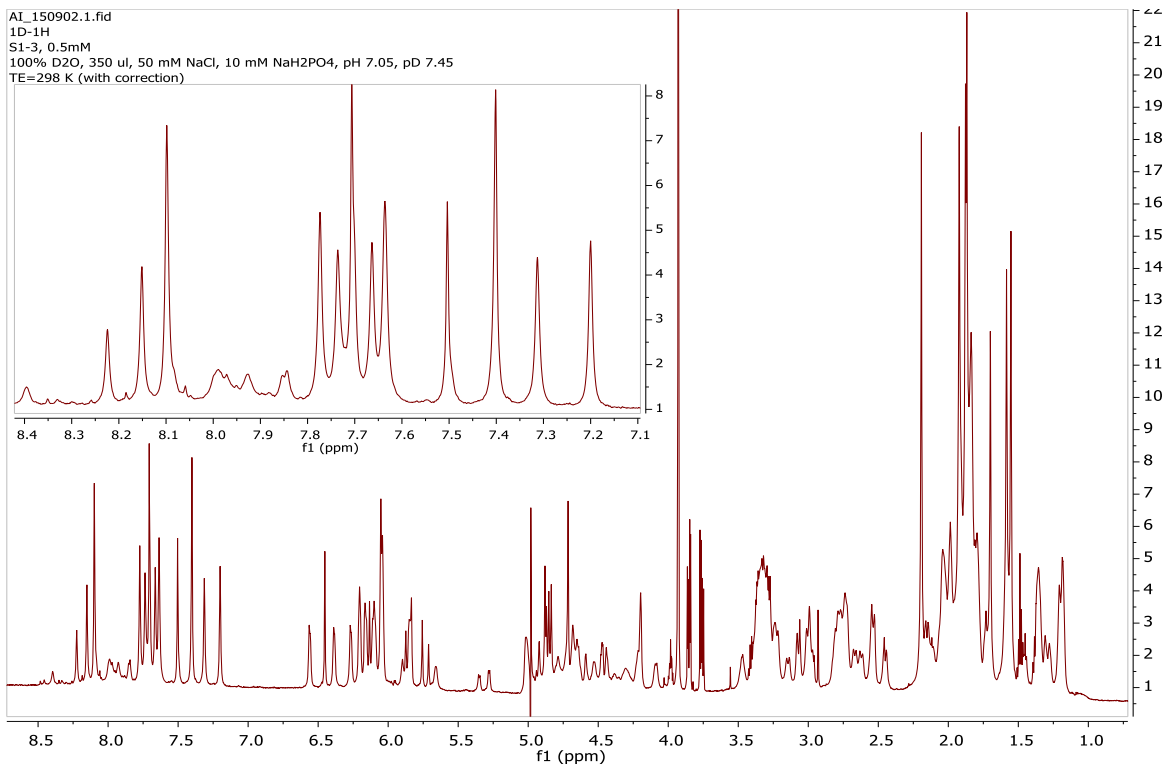


Figure S3. One-dimensional NMR spectrum of tc-DNA•RNA duplex in D2O at 298 K.

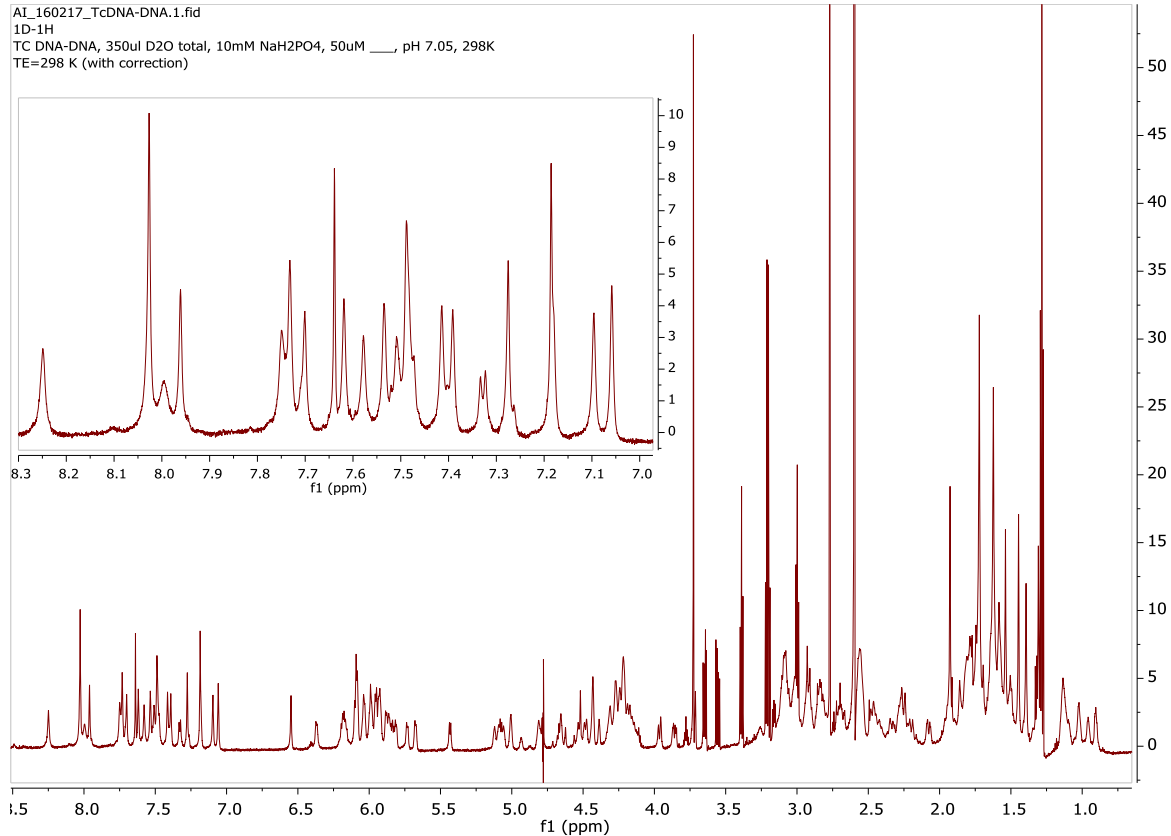


Figure S4. One-dimensional NMR spectrum of tc-DNA•DNA duplex in D2O at 298 K.

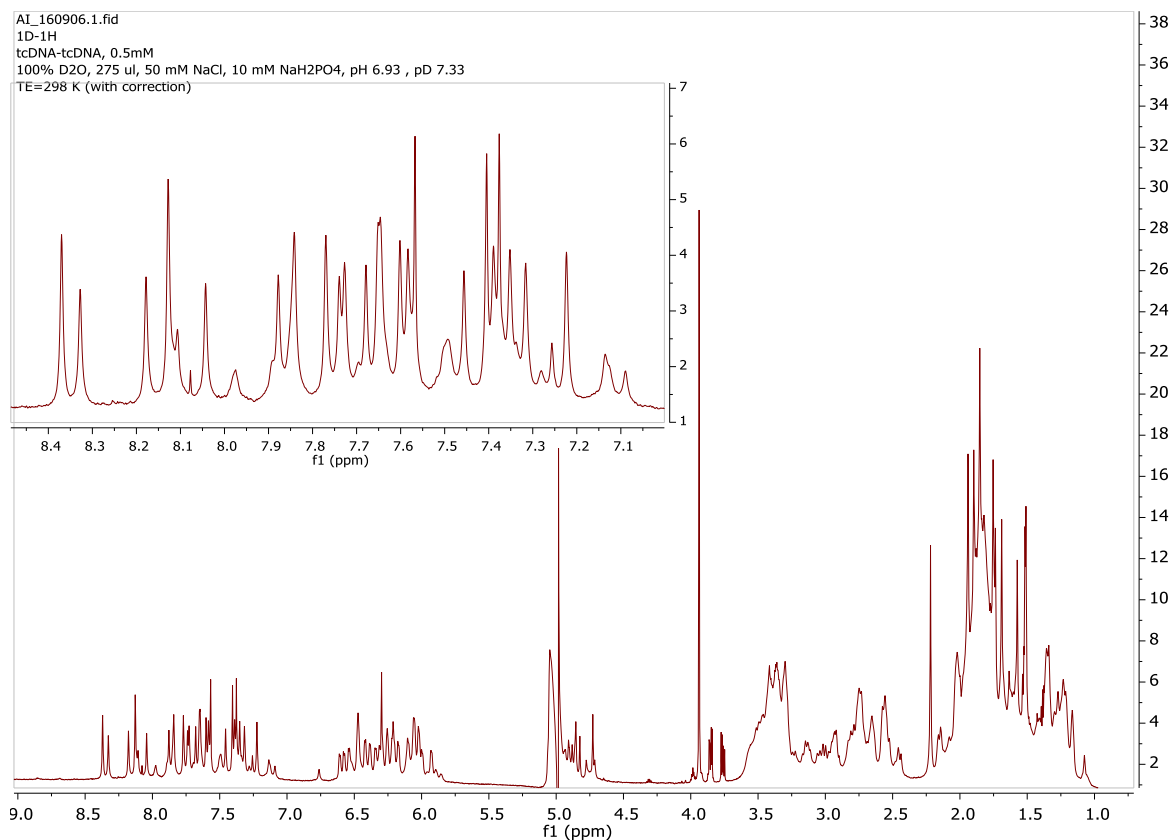


Figure S5. One-dimensional NMR spectrum of tc-DNA•tc-DNA duplex in D2O at 298 K.

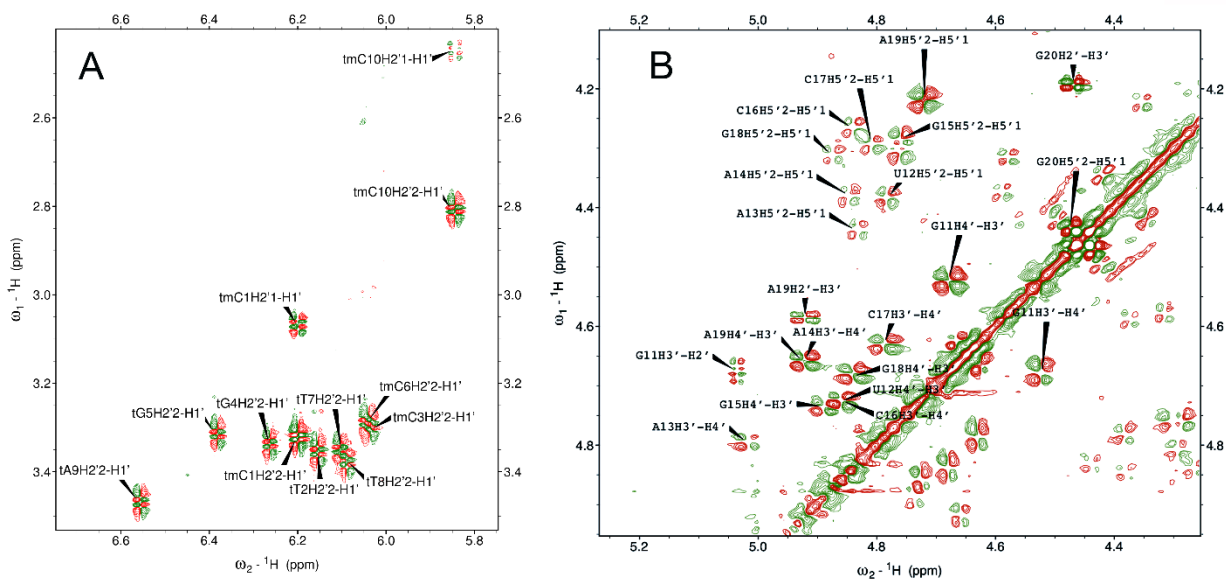


Figure S6. Expanded DQF-COSY spectrum of tc-DNA•RNA duplex, showing (A) strong H2'2'-H1' and very weak H2'1'-H1' (peaks are missing) coupling constants of tc-DNA sugars and (B) strong H3'-4' and very weak H1'-H2' (peaks are missing) coupling constants of RNA sugars. The observed peaks are consistent with Northern sugar conformation.

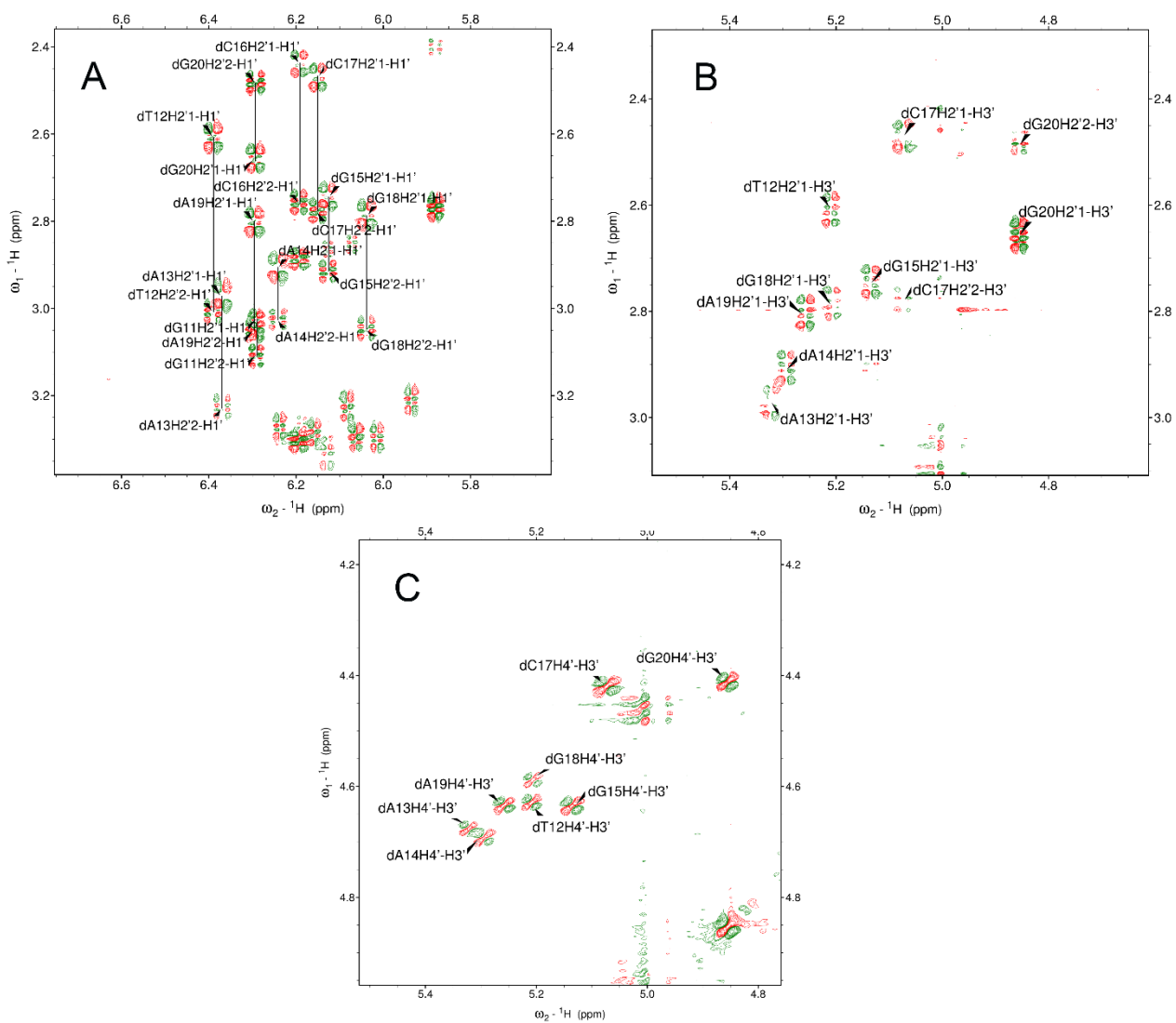


Figure S7. Expanded DQF-COSY spectrum of tc-DNA•DNA duplex, illustrating (A) strong H2'1 -H1', medium H2'2-H1', (B) undetectable H2'2-3' (peaks are missing) and (C) medium H4'-H3' coupling constants of DNA sugars. The observed peaks are consistent with the existence of a South-East-North deoxyribose conformation equilibrium.

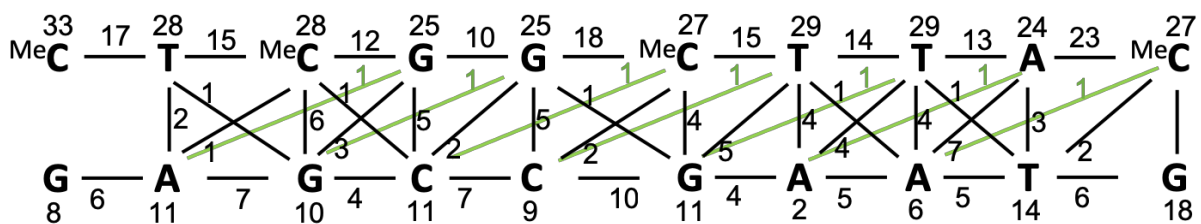
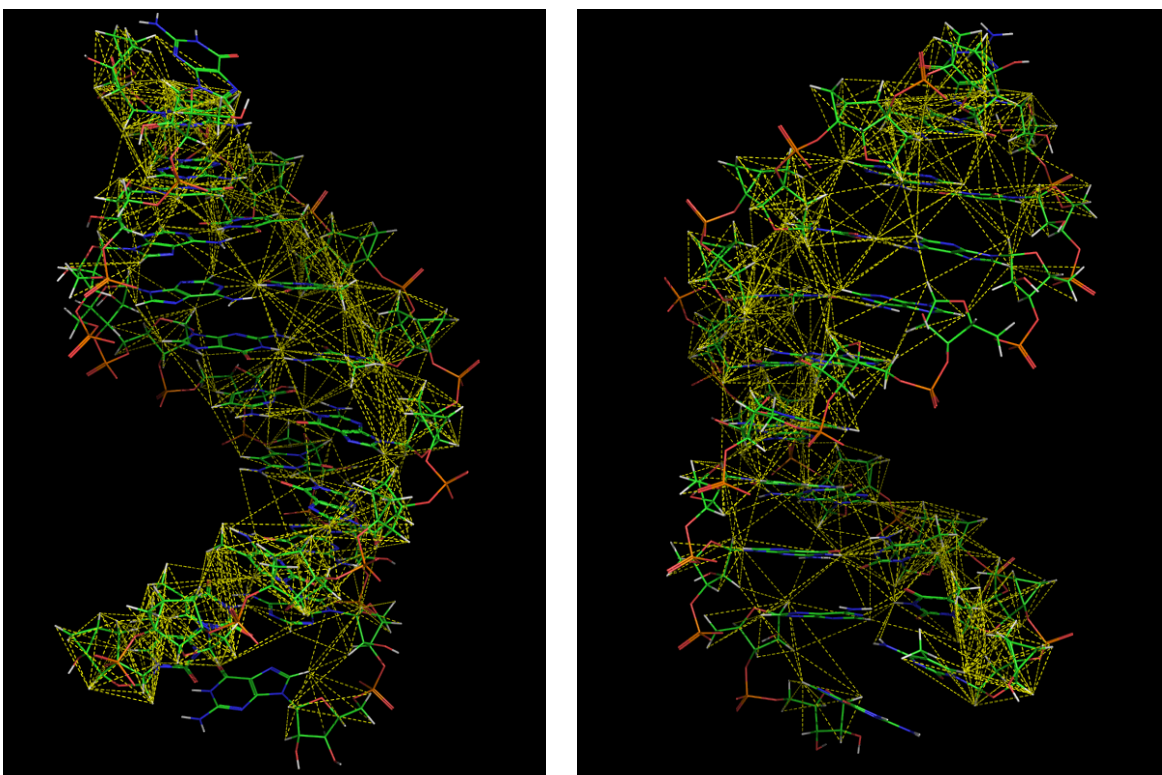


Figure S8. The distribution of the NOE restraints obtained from RANDMARDI calculations for Tc-DNA•RNA duplex

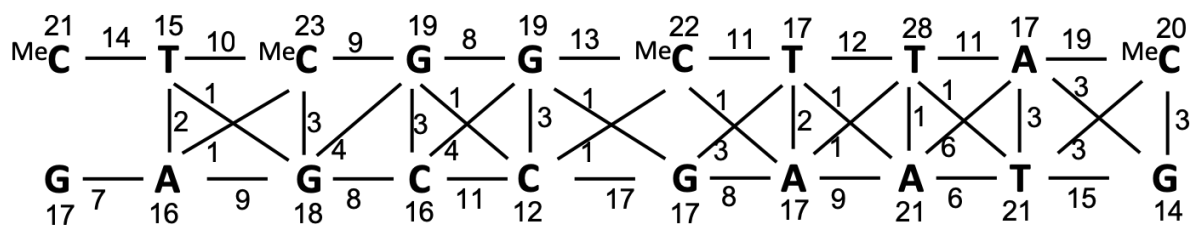
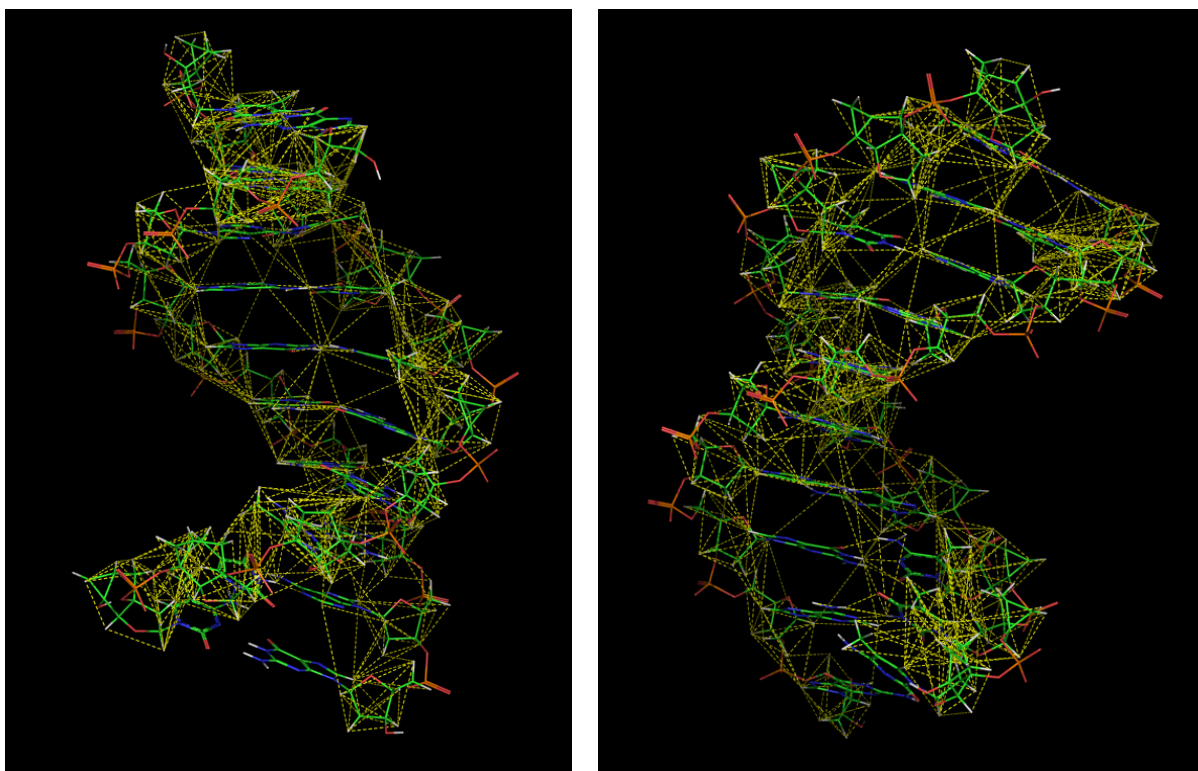


Figure S9. The distribution of the NOE restraints obtained from RANDMARDI calculations for Tc-DNA•DNA duplex.

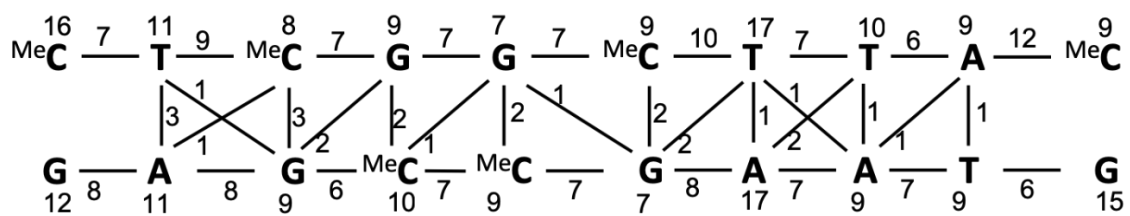
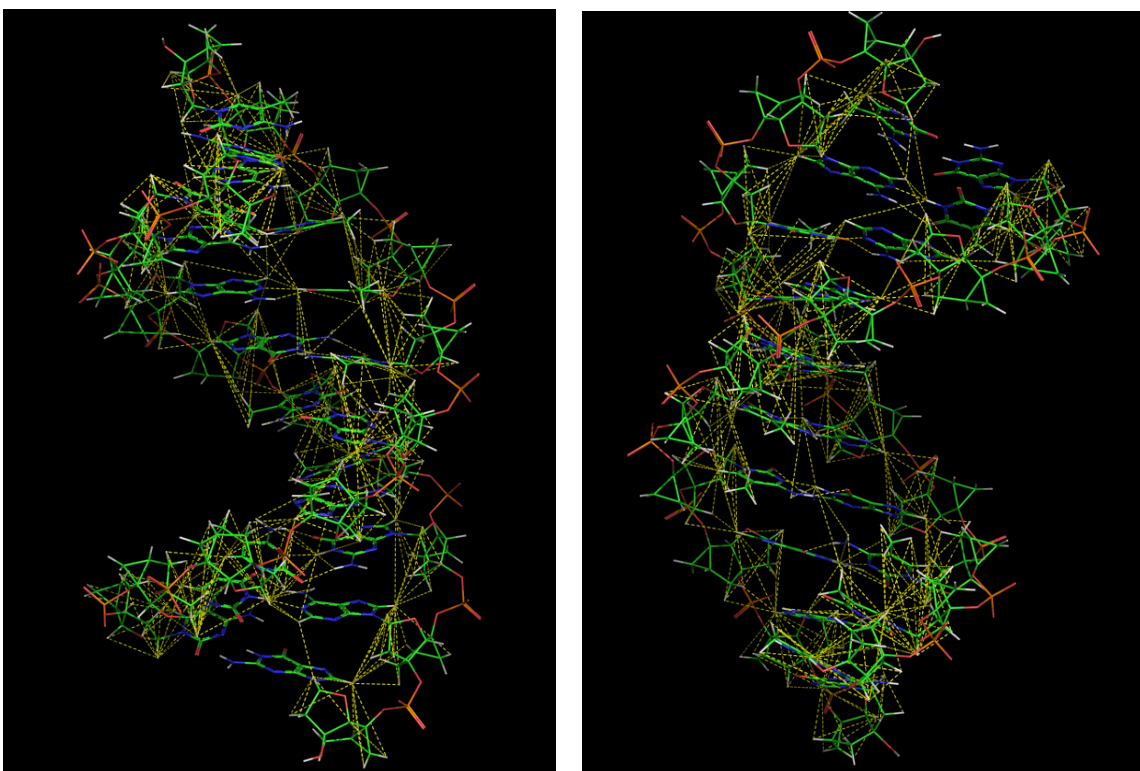


Figure S10. The distribution of the NOE restraints obtained from RANDMARDI calculations for tc-DNA•tc-DNA duplex.

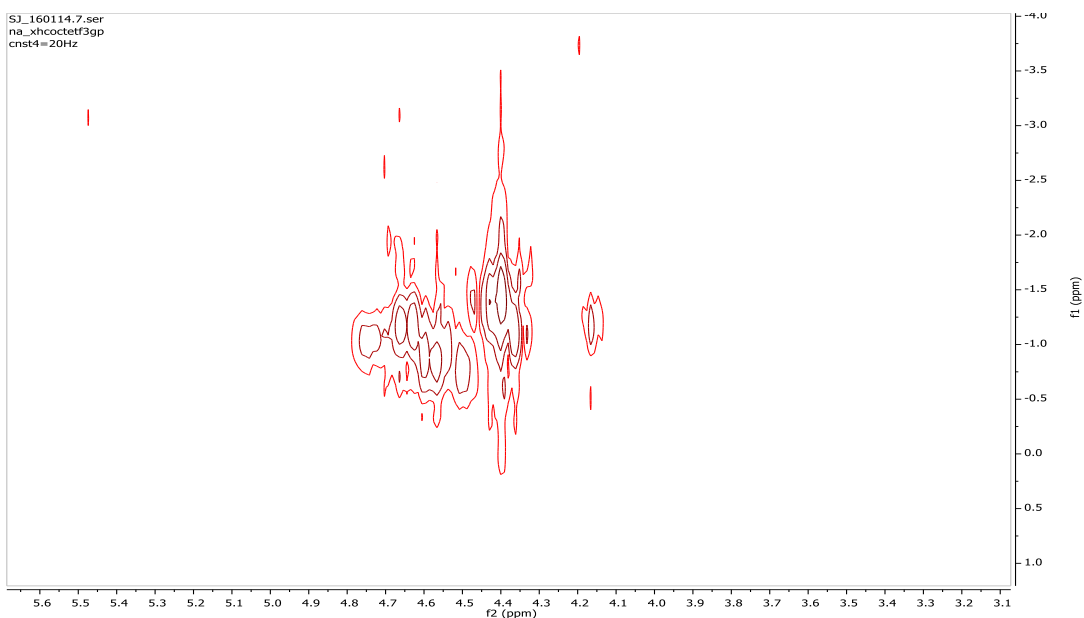


Figure S11. Expanded ^1H - ^{31}P HETCOR spectrum of tc-DNA•RNA.

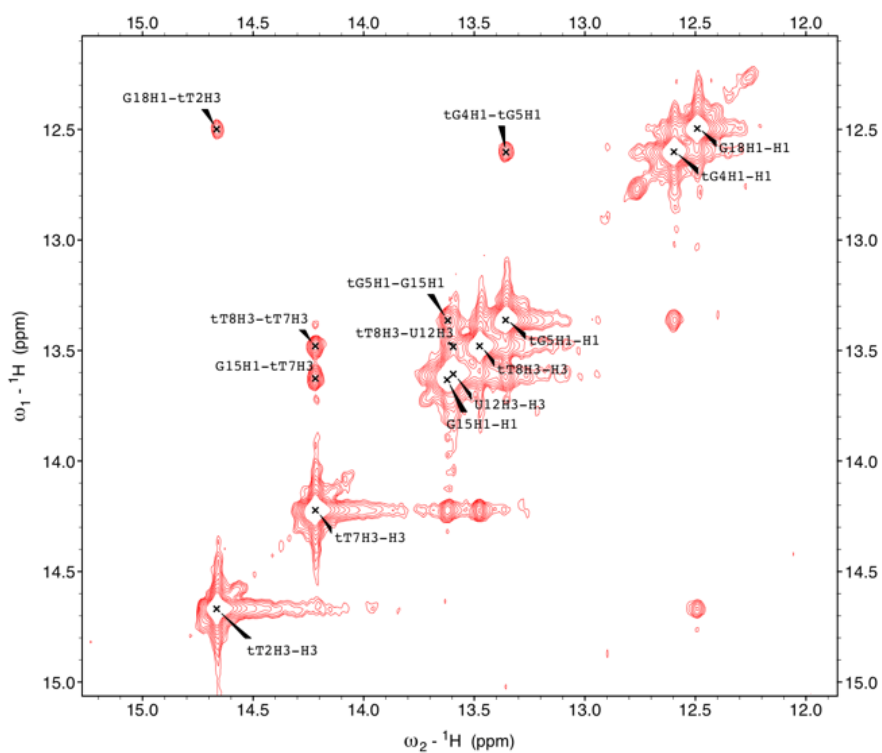


Figure S12. Diagonal imino region of the 250 ms NOESY spectrum of tc-DNA•RNA duplex recorded at 283 K.

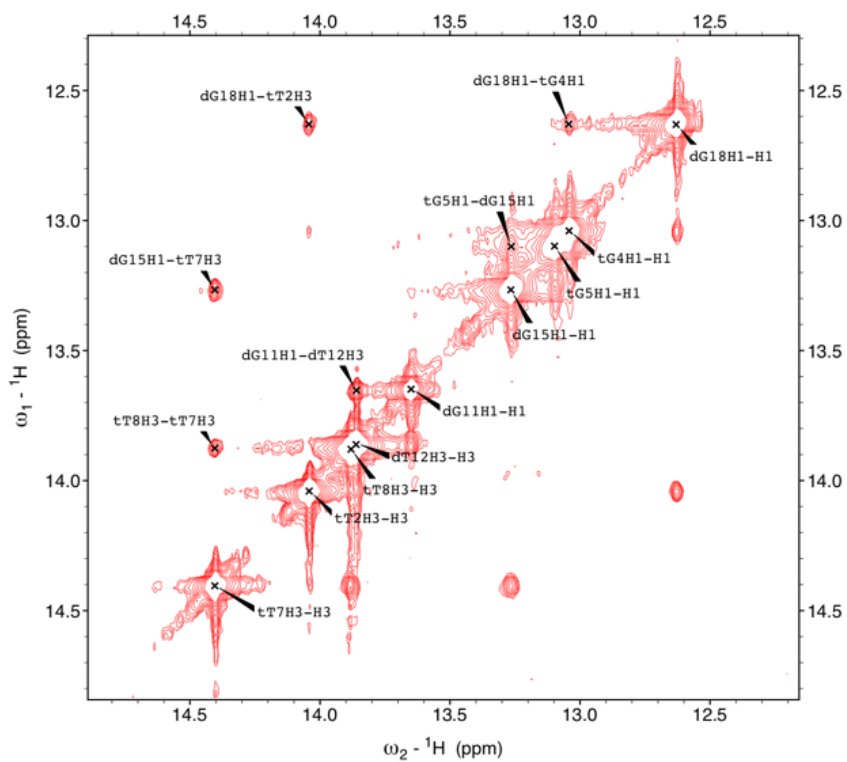


Figure S13. Diagonal imino region of the 250 ms NOESY spectrum of tc-DNA•DNA duplex recorded at 283 K.

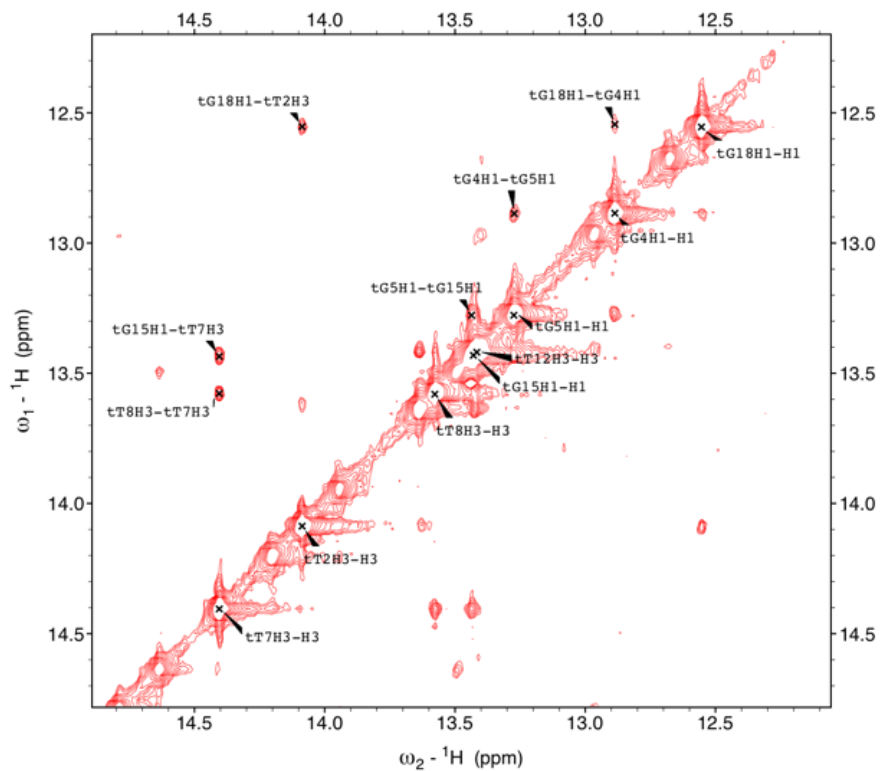


Figure S14. Diagonal imino region of the 250 ms NOESY spectrum of tc-DNA•tc-DNA duplex recorded at 283 K.

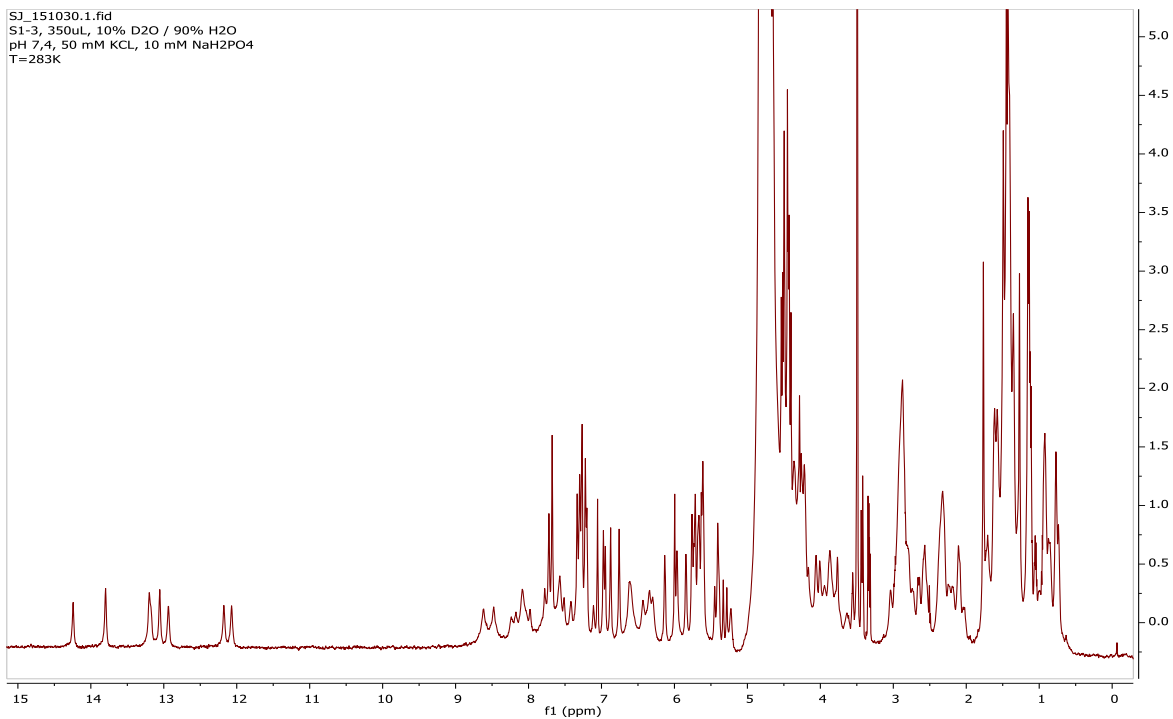


Figure S15. One-dimensional NMR spectrum of tc-DNA•RNA duplex in H₂O at 283 K.

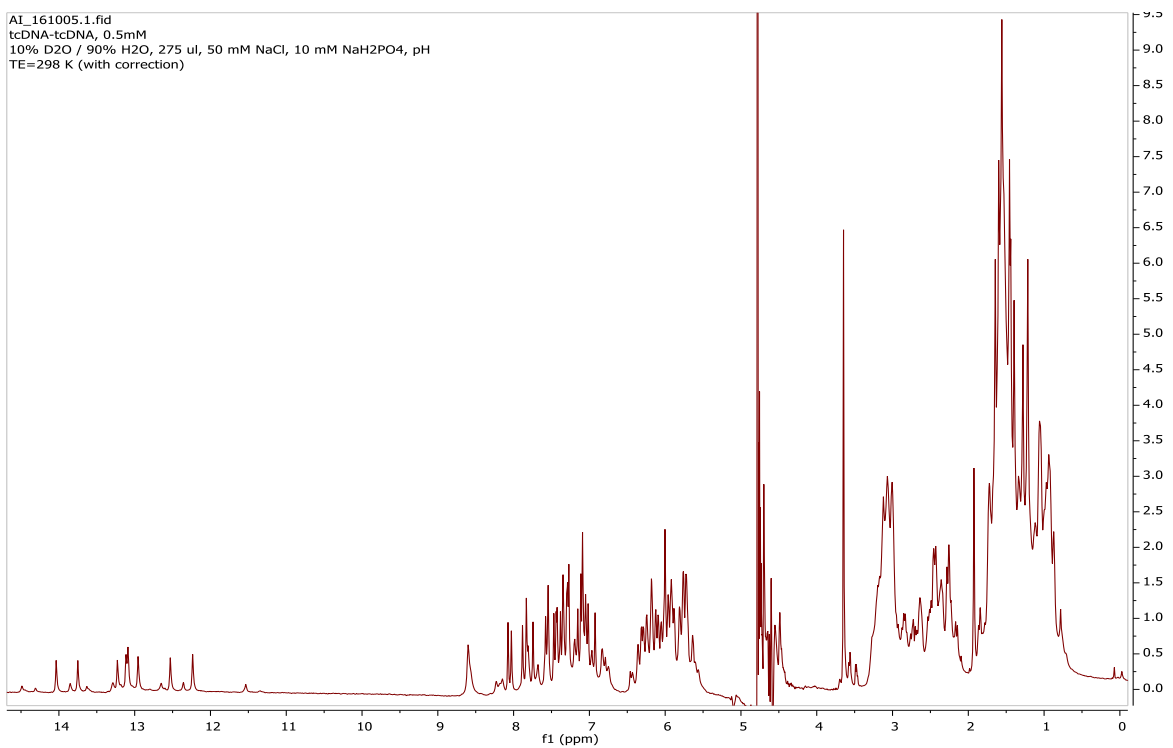


Figure S16. One-dimensional NMR spectrum of tc-DNA•tc-DNA duplex in H₂O at 283 K.

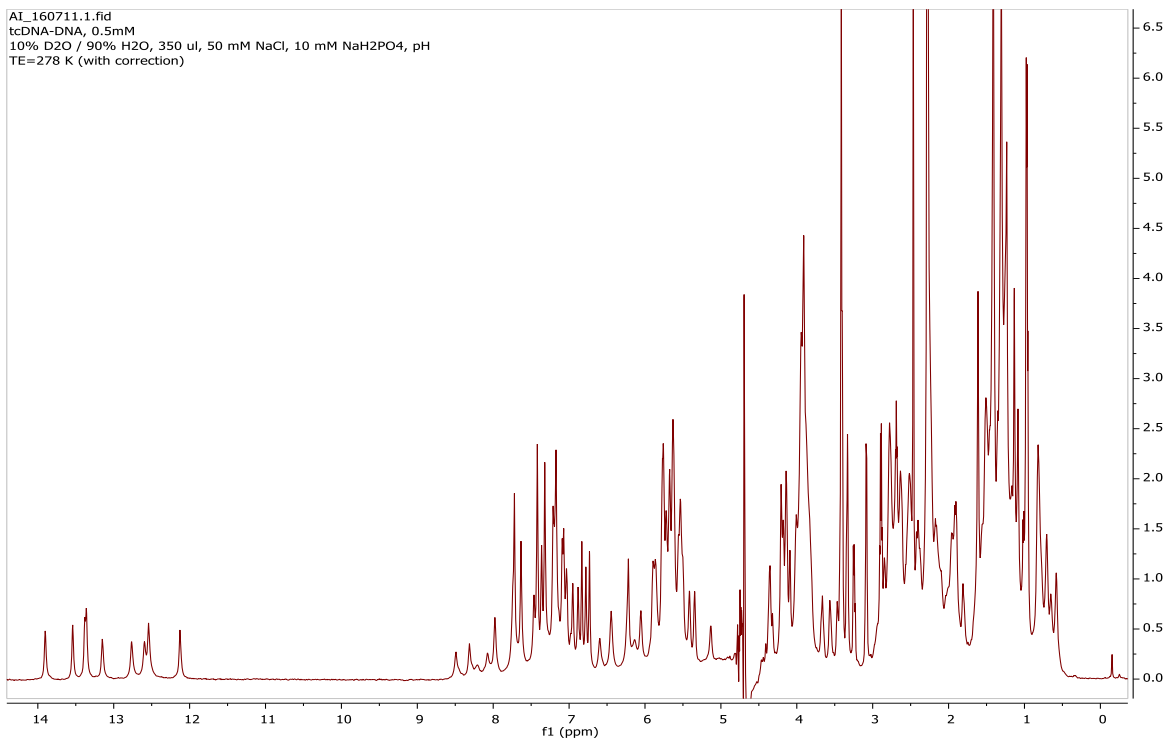


Figure S17. One-dimensional NMR spectrum of tc-DNA•DNA duplex in H₂O at 283 K.

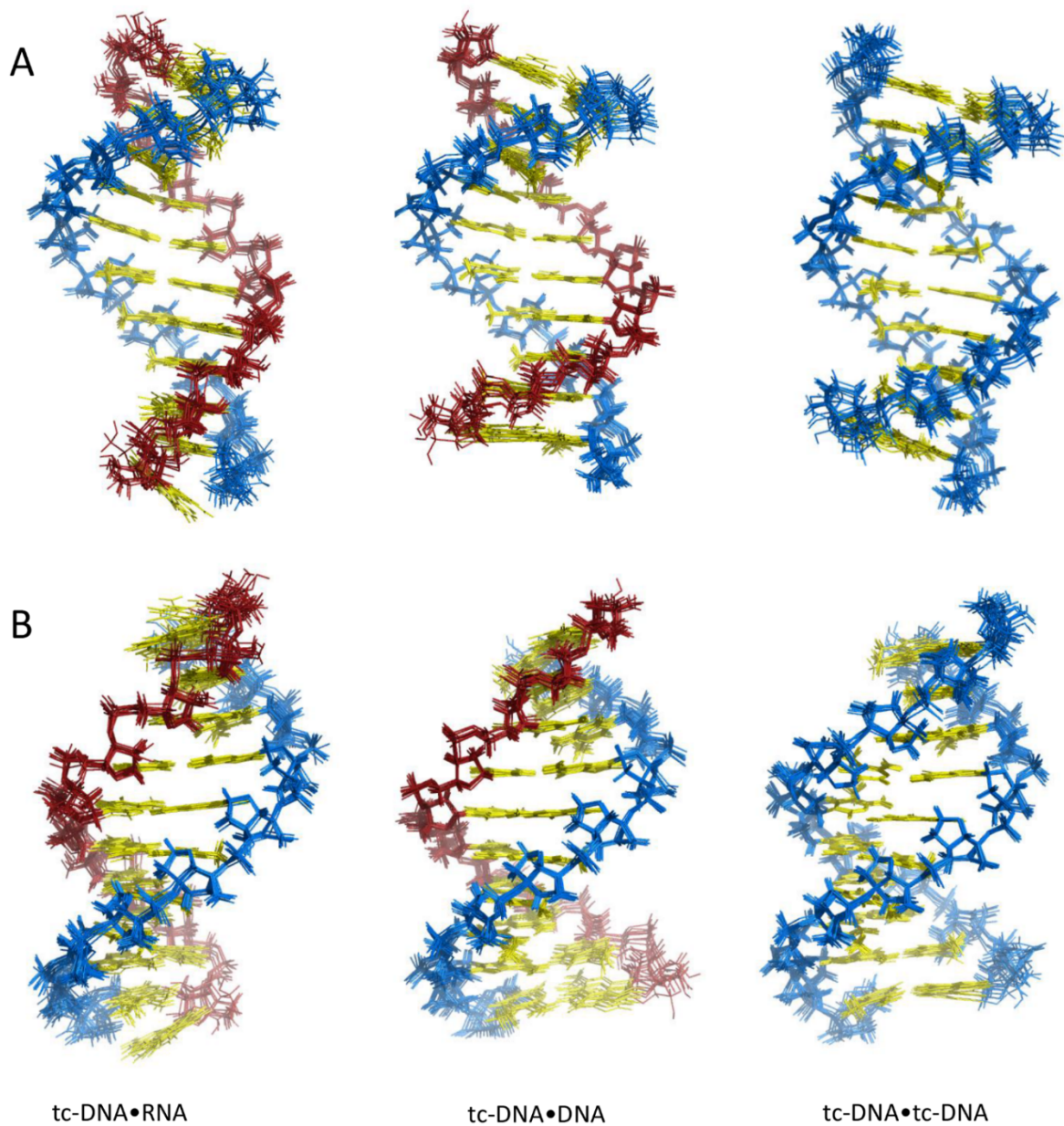


Figure S18. Comparison of the tc-DNA•RNA, tc-DNA•DNA, and tc-DNA•tc-DNA ensembles of 10 structures with lowest NOE energy. **(A)** View from the major groove. **(B)** View from the minor groove. The nucleobases are shown in yellow, tc-DNA sugar-phosphate backbone in blue and DNA/RNA sugar-phosphate backbone in red.

Table S1. Nonexchangeable ¹H chemical shifts for tc-DNA•RNA duplex at 25 °C.

Residue	H1'	H2	H2'	H2'1	H2'2	H3'	H4'	H5	H5'1	H5'2	H6	H6'	H7'1	H7'2	H7*	H8	H8'1	H8'2
tmC1	6.20	-	-	3.07	3.32	-	4.85	-	-	-	8.10	1.92	2.15	2.54	2.19	-	1.18	1.82
tT2	6.16	-	-	3.26	3.35	-	4.92	-	-	-	7.77	2.04	2.06	2.78	1.86	-	1.36	1.84
tmC3	6.04	-	-	2.98	3.30	-	4.92	-	-	-	7.66	1.99	2.03	2.62	1.92	-	1.34	1.79
tG4	6.27	-	-	3.22	3.34	-	4.88	-	-	-	-	1.84	1.57	2.54	-	7.70	1.20	1.78
tG5	6.38	-	-	3.23	3.32	-	4.88	-	-	-	-	1.78	1.45	2.73	-	7.40	1.21	1.83
tmC6	6.05	-	-	3.00	3.29	-	4.83	-	-	-	7.31	1.89	1.86	2.67	1.58	-	1.30	1.80
tT7	6.10	-	-	3.14	3.35	-	4.87	-	-	-	7.63	1.99	1.98	2.77	1.70	-	1.35	1.86
tT8	6.09	-	-	3.00	3.38	-	4.94	-	-	-	7.73	2.02	2.11	2.74	1.88	-	1.36	1.84
tA9	6.56	7.40	-	3.29	3.47	-	4.71	-	-	-	-	1.91	1.59	2.73	-	8.15	1.27	1.87
tmC10	5.85	-	-	2.45	2.81	-	4.71	-	-	-	7.20	1.83	1.86	1.93	1.55	-	1.18	1.73
G11	5.89	-	5.04	-	-	4.67	4.52	-	4.20	4.08	-	-	-	-	-	8.21	-	-
U12	5.83	-	4.68	-	-	4.86	4.73	5.35	4.79	4.38	8.08	-	-	-	-	-	-	-
A13	6.17	6.45	n.a.	-	-	4.79	5.01	-	4.84	4.44	-	-	-	-	-	8.39	-	-
A14	6.04	7.50	4.91	-	-	4.65	4.92	-	4.84	4.38	-	-	-	-	-	7.97	-	-
G15	5.83	-	4.67	-	-	4.89	4.73	-	4.77	4.28	-	-	-	-	-	7.50	-	-
C16	5.75	-	4.65	-	-	4.72	4.85	5.28	4.85	4.27	7.85	-	-	-	-	-	-	-
C17	5.71	-	4.89	-	-	4.63	4.79	5.66	4.81	4.30	7.99	-	-	-	-	-	-	-
G18	5.87	-	4.78	-	-	4.84	4.68	-	4.88	4.31	-	-	-	-	-	7.72	-	-
A19	6.13	7.70	4.59	-	-	4.92	4.66	-	4.73	4.22	-	-	-	-	-	7.93	-	-
G20	6.05	-	4.24	-	-	4.47	4.73	-	4.47	4.43	-	-	-	-	-	7.63	-	-

n.a – not assigned.

Table S2. Exchangeable ¹H chemical shifts for tc-DNA•RNA duplex at 10 °C.

Residue	H1	H21	H22	H3	H41	H42	H61	H62
tmC1	-	-	-	-	8.6	7.05	-	-
tT2	-	-	-	14.66	-	-	-	-
tmC3	-	-	-	-	8.9	6.73	-	-
tG4	12.6	8.46	5.98	-	-	-	-	-
tG5	13.36	8.43	6.05	-	-	-	-	-
tmC6	-	-	-	-	9.04	6.77	-	-
tT7	-	-	-	14.22	-	-	-	-
tT8	-	-	-	13.48	-	-	-	-
tA9	-	-	-	-	-	-	8.19	6.39
tmC10	-	-	-	-	8.67	6.86	-	-
G11	13.28	n.a.	n.a.	-	-	-	-	-
U12	-	-	-	13.59	-	-	-	-
A13	-	-	-	-	-	-	8.04	6.81
A14	-	-	-	-	-	-	8.16	6.8
G15	13.62	n.a.	n.a.	-	-	-	-	-
C16	-	-	-	-	8.5	7.03	-	-
C17	-	-	-	-	8.51	7.02	-	-
G18	12.49	n.a.	n.a.	-	-	-	-	-
A19	-	-	-	-	-	-	8.60	7.05
G20	n.a.	n.a.	n.a.	-	-	-	-	-

n.a – not assigned.

Table S3. ¹³C chemical shifts for tc-DNA•RNA duplex at 25 °C.

Residue	C1'	C2	C2'	C3'	C4'	C5	C5'	C6	C6'	C7'	C8	C8'
tmC1	90.67	-	n.a.	n.a.	93.62	-	n.a.	140.7	25.64	42.28	-	18.42
tT2	91.96	-	n.a.	n.a.	93.4	-	n.a.	138.4	25.48	41.96	-	17.33
tmC3	91.74	-	n.a.	n.a.	93.39	-	n.a.	137.9	25.25	40.47	-	17.17
tG4	90.69	-	n.a.	n.a.	93.34	-	n.a.	-	25.69	41.06	136.3	17.17
tG5	90.89	-	n.a.	n.a.	93.15	-	n.a.	-	25.43	41.7	136.3	17.2
tmC6	90.83	-	n.a.	n.a.	92.8	-	n.a.	137.9	24.82	41.34	-	16.99
tT7	91.96	-	n.a.	n.a.	93.57	-	n.a.	137.9	25.69	41.86	-	17.23
tT8	91.92	-	n.a.	n.a.	93.42	-	n.a.	137.6	25.48	40.58	-	17.3
tA9	91.14	153.1	n.a.	n.a.	92.62	-	n.a.	-	25.64	42.33	139.8	17.3
tmC10	90.97	-	49.95	n.a.	91.88	-	n.a.	137.9	25.5	42.39	-	17.16
G11	93.25	-	74.97	72.67	84.73	-	n.a.	-	-	-	139	-
U12	93.95	-	74	72.63	n.a.	102.4	64.87	142.2	-	-	-	-
A13	92.94	151.9	n.a.	71.88	82.08	-	65.14	-	-	-	140	-
A14	92.73	153.3	75.46	n.a.	n.a.	-	64.8	-	-	-	-	-
G15	92.94	-	73.79	72.9	82.06	-	64.9	-	-	-	135.8	-
C16	94.11	-	75.14	n.a.	n.a.	96.55	64.21	141.1	-	-	-	-
C17	93.89	-	74.94	71.87	82.19	97.63	64.11	140.8	-	-	-	-
G18	93.16	-	75.08	72.56	82.03	-	64.3	-	-	-	136.3	-
A19	93.33	153.6	75.56	72.37	82.25	-	65.68	-	-	-	139.4	-
G20	-	-	76.44	70.58	n.a.	-	70.57	-	-	-	137.2	-

n.a – not assigned.

Table S4. Nonexchangeable ¹H chemical shifts for tc-DNA•DNA duplex at 25 °C.

Residue	H1'	H2	H2'1	H2'2	H3'	H4'	H5	H5'1	H5'2	H6	H6'	H7'1	H7'2	H7*	H8	H8'1	H8'2
tmC1	6.19	-	2.88	3.30	-	4.73	-	-	-	7.93	1.93	2.28	2.45	2.13	-	1.11	1.82
tT2	6.06	-	2.88	3.29	-	4.87	-	-	-	7.69	2.01	2.00	2.75	1.82	-	1.33	1.78
tmC3	6.08	-	3.18	3.22	-	4.91	-	-	-	7.62	2.02	2.10	2.63	1.92	-	1.33	1.78
tG4	6.16	-	3.21	3.29	-	4.88	-	-	-	-	1.92	1.72	2.54	-	7.71	1.22	1.78
tG5	6.24	-	3.14	3.27	-	4.86	-	-	-	-	1.92	1.54	2.67	-	7.38	1.22	1.78
tmC6	5.94	-	3.12	3.21	-	4.83	-	-	-	7.30	1.90	1.80	2.68	1.59	-	1.29	1.77
tT7	6.01	-	3.13	3.30	-	4.85	-	-	-	7.59	2.00	1.95	2.76	1.74	-	1.33	n.a.
tT8	6.13	-	3.13	3.34	-	4.94	-	-	-	7.74	2.06	2.16	2.76	1.93	-	1.34	1.82
tA9	6.57	7.39	3.27	3.46	-	n.a.	-	-	-	-	1.99	1.71	2.74	-	8.16	1.31	1.84
tmC10	5.88	-	2.40	2.77	-	4.72	-	-	-	7.26	1.84	n.a.	1.97	1.65	-	1.16	1.70
dG11	6.29	-	3.03	3.10	n.a.	4.47	-	4.16	4.06	-	-	-	-	-	8.23	-	-
dT12	6.39	-	2.61	3.01	5.21	4.63	-	4.42	4.42	7.82	-	-	-	1.51	-	-	-
dA13	6.37	6.75	2.97	3.23	5.32	4.68	-	4.38	4.52	-	-	-	-	-	8.45	-	-
dA14	6.24	7.48	2.91	3.03	5.29	4.69	-	4.51	4.51	-	-	-	-	-	8.20	-	-
dG15	6.13	-	2.75	2.92	5.14	4.63	-	4.47	4.47	-	-	-	-	-	7.78	-	-
dC16	6.19	-	2.44	2.76	n.a.	4.45	5.28	4.48	4.38	7.53	-	-	-	-	-	-	-
dC17	6.15	-	2.47	2.78	5.07	4.42	5.63	4.36	4.36	7.68	-	-	-	-	-	-	-
dG18	6.04	-	2.79	3.04	5.21	4.59	-	4.32	4.40	-	-	-	-	-	7.95	-	-
dA19	6.30	7.84	2.80	3.05	5.26	4.64	-	4.42	4.46	-	-	-	-	-	8.23	-	-
dG20	6.29	-	2.66	2.48	4.86	4.41	-	4.35	4.43	-	-	-	-	-	7.90	-	-

n.a – not assigned.

Table S5. Exchangeable ¹H chemical shifts for tc-DNA•DNA duplex at 10 °C.

Residue	H1	H3	H41	H42	H61	H62
tmC1	-	-	n.a.	n.a.	-	-
tT2	-	14.04	-	-	-	-
tmC3	-	-	8.991	6.737	-	-
tG4	13.04	-	-	-	-	-
tG5	13.1	-	-	-	-	-
tmC6	-	-	8.718	6.728	-	-
tT7	-	14.4	-	-	-	-
tT8	-	13.88	-	-	-	-
tA9	-	-	-	-	8.477	6.62
tmC10	-	-	8.815	6.943	-	-
dG11	13.65	-	-	-	-	-
dT12	-	13.86	-	-	-	-
dA13	-	-	-	-	8.135	6.489
dA14	-	-	-	-	8.023	6.439
dG15	13.27	-	-	-	-	-
dC16	-	-	8.229	6.635	-	-
dC17	-	-	8.578	6.947	-	-
dG18	12.63	-	-	-	-	-
dA19	-	-	-	-	8.207	6.345
tA19	-	-	-	-	n.a.	n.a.
dG20	n.a.	n.a.	-	-	-	-

n.a – not assigned.

Table S6. ¹³C chemical shifts for tc-DNA•DNA duplex at 25 °C.

Residue	C1'	C2'	C3'	C4'	C5	C5'	C6'	C7'	C8'
tmC1	89.61	45.75	n.a.	92.96	n.a.	n.a.	25.8	42.52	18.97
tT2	91.88	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
tmC3	91.85	n.a.	n.a.	93.41	n.a.	n.a.	n.a.	40.83	n.a.
tG4	90.52	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	41.31	n.a.
tG5	90.67	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
tmC6	92.00	n.a.	n.a.	92.91	n.a.	n.a.	24.88	n.a.	n.a.
tT7	92.00	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
tT8	91.76	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
tA9	90.99	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
tmC10	90.80	49.88	n.a.	91.97	n.a.	n.a.	25.44	n.a.	n.a.
dG11	87.53	n.a.	n.a.	88.32	n.a.	63.15	-	-	-
dT12	86.27	n.a.	79.72	87.01	n.a.	n.a.	-	-	-
dA13	84.80	n.a.	79.39	87.09	n.a.	n.a.	-	-	-
dA14	84.23	n.a.	78.09	86.88	n.a.	68.09	-	-	-
dG15	84.85	n.a.	77.92	n.a.	n.a.	68.09	-	-	-
dC16	86.67	n.a.	n.a.	85.45	97.33	66.94	-	-	-
dC17	86.64	n.a.	77.09	n.a.	98.27	67.16	-	-	-
dG18	84.68	n.a.	79.97	87.10	n.a.	68.38	-	-	-
dA19	84.78	n.a.	78.64	86.65	n.a.	n.a.	-	-	-
dG20	84.44	n.a.	72.93	87.69	n.a.	n.a.	-	-	-

n.a – not assigned

Table S7. Nonexchangeable ¹H chemical shifts for tc-DNA•tc-DNA duplex at 25 °C.

Residue	H1'	H2	H2'1	H2'2	H4'	H6	H6'	H7'1	H7'2	H7*	H8	H8'1	H8'2
tmC1	6.25	-	3.01	3.34	4.85	8.12	1.95	2.15	2.56	2.22	-	1.20	1.85
tT2	6.17	-	3.38	3.35	n.a.	7.76	n.a.	2.03	2.77	1.85	-	n.a.	n.a.
tmC3	6.02	-	3.12	3.29	n.a.	7.65	n.a.	2.07	2.65	1.94	-	n.a.	n.a.
tG4	6.21	-	3.27	3.35	n.a.	-	n.a.	1.62	2.56	-	7.74	n.a.	n.a.
tG5	6.38	-	3.31	3.34	n.a.	-	n.a.	1.56	2.73	-	7.45	n.a.	n.a.
tmC6	6.06	-	3.05	3.30	4.86	7.35	n.a.	1.90	2.74	1.57	-	n.a.	n.a.
tT7	6.10	-	3.15	3.36	4.88	7.64	n.a.	1.98	2.81	1.73	-	1.35	2.01
tT8	6.02	-	2.93	3.37	n.a.	7.72	n.a.	2.12	2.74	1.89	-	n.a.	n.a.
tA9	6.57	7.37	3.29	3.46	n.a.	-	n.a.	1.61	2.73	-	8.17	n.a.	n.a.
tmC10	5.92	-	2.44	2.80	4.72	7.22	n.a.	2.44	2.80	1.51	-	n.a.	n.a.
tG11	6.47	-	3.31	3.41	4.93	-	1.91	1.75	2.53	-	8.37	1.16	1.68
tT12	6.20	-	3.50	3.41	n.a.	7.60	n.a.	2.15	2.70	1.69	-	n.a.	n.a.
tA13	6.54	6.29	3.38	3.57	n.a.	-	n.a.	1.76	2.66	-	8.32	n.a.	n.a.
tA14	6.47	7.40	3.41	3.47	n.a.	-	n.a.	1.67	2.57	-	7.87	n.a.	n.a.
tG15	6.34	-	3.29	3.35	n.a.	-	n.a.	1.61	2.77	-	7.39	n.a.	n.a.
tmC16	6.05	-	2.96	3.30	4.85	7.31	n.a.	1.94	2.75	1.51	-	n.a.	n.a.
tmC17	5.99	-	3.14	3.30	4.86	7.58	n.a.	2.08	2.65	1.75	-	n.a.	n.a.
tG18	6.29	-	3.23	3.42	n.a.	-	n.a.	1.76	2.64	-	7.84	n.a.	n.a.
tA19	6.60	7.56	3.43	3.50	n.a.	-	1.86	1.77	2.56	-	8.04	1.25	1.86
tG20	6.42	-	2.92	2.94	4.82	-	1.68	n.a.	n.a.	-	7.68	1.07	1.74

n.a – not assigned

Table S8. Exchangeable ¹H chemical shifts for tc-DNA•tc-DNA duplex at 10 °C.

Residue	H1	H21	H22	H3	H41	H42	H61	H62
tmC1	-	-	-	-	n.a.	n.a.	-	-
tT2	-	-	-	14.09	-	-	-	-
tmC3	-	-	-	-	8.901	6.744	-	-
tG4	12.89	n.a.	n.a.	-	-	-	-	-
tG5	13.27	n.a.	n.a.	-	-	-	-	-
tmC6	-	-	-	-	8.904	6.767	-	-
tT7	-	-	-	14.4	-	-	-	-
tT8	-	-	-	13.58	-	-	-	-
tA9	-	-	-	-	-	-	n.a.	n.a.
tmC10	-	-	-	-	n.a.	n.a.	-	-
tG11	n.a.	n.a.	n.a.	-	-	-	-	-
tT12	-	-	-	13.42	-	-	-	-
tA13	-	-	-	-	-	-	n.a.	n.a.
tA14	-	-	-	-	-	-	n.a.	n.a.
tG15	13.44	n.a.	n.a.	-	-	-	-	-
tmC16	-	-	-	-	8.893	6.753	-	-
tmC17	-	-	-	-	8.891	6.684	-	-
tG18	12.55	7.635	n.a.	-	-	-	-	-
tA19	-	-	-	-	-	-	8.489	6.484
tG20	n.a.	n.a.	n.a.	-	-	-	-	-

n.a – not assigned

AMBER forcefield parameters used for the modified nucleotides

The partial charges were derived from QM calculations at HF/6-31G* theory level with the GAUSSIAN 09 (1) and fitted to each atomic centre with R.E.D.-III.5 (2) tools program package according to the RESP (3) algorithm. Three new atom types were introduced to account for the three-membered ring in tricyclo-DNA: C8, C6, C5. The bond length angle values for the new atom types were derived from QM calculations at HF/6-31G* theory level with the GAUSSIAN 09. The Kr and K_o were assigned by analogy with similar atom types. This is a good approximation for the restrained MD calculations performed in this research but might be not accurate enough for unrestrained MD calculations.

RESI TA ! Tc-ADENOSINE

GROUP

```
ATOM P TYPE=P CHARGE= 1.21660 END !
ATOM O1P TYPE=O2 CHARGE=-0.79140 END !
ATOM O2P TYPE=O2 CHARGE=-0.79140 END !
ATOM O5' TYPE=OS CHARGE=-0.49280 END !
ATOM C5' TYPE=C5 CHARGE= 0.20640 END !
ATOM C4' TYPE=CT CHARGE= 0.19590 END !
ATOM H4' TYPE=H1 CHARGE= 0.09370 END !
ATOM O4' TYPE=OS CHARGE=-0.45460 END !
ATOM C1' TYPE=CT CHARGE= 0.16710 END !
ATOM H1' TYPE=H2 CHARGE= 0.09440 END !
ATOM N9 TYPE=N* CHARGE=-0.01910 END !
ATOM C8 TYPE=CK CHARGE= 0.19630 END !
ATOM H8 TYPE=H5 CHARGE= 0.14300 END !
ATOM N7 TYPE=NB CHARGE=-0.59160 END !
ATOM C5 TYPE=CB CHARGE= 0.02890 END !
ATOM C6 TYPE=CA CHARGE= 0.67280 END !
ATOM N6 TYPE=N2 CHARGE=-0.87840 END !
ATOM H61 TYPE=H CHARGE= 0.39800 END !
ATOM H62 TYPE=H CHARGE= 0.39800 END !
ATOM N1 TYPE=NC CHARGE=-0.75700 END !
ATOM C2 TYPE=CQ CHARGE= 0.60020 END !
ATOM H2 TYPE=H5 CHARGE= 0.04740 END !
ATOM N3 TYPE=NC CHARGE=-0.75770 END !
ATOM C4 TYPE=CB CHARGE= 0.39800 END !
ATOM C3' TYPE=CT CHARGE= 0.27860 END !
ATOM C2' TYPE=CT CHARGE=-0.07600 END !
ATOM H2'1 TYPE=HC CHARGE= 0.05590 END !
ATOM H2'2 TYPE=HC CHARGE= 0.05590 END !
ATOM C7' TYPE=CT CHARGE=-0.10070 END !
ATOM H7'1 TYPE=HC CHARGE= 0.04060 END !
ATOM H7'2 TYPE=HC CHARGE= 0.04060 END !
ATOM C6' TYPE=C6 CHARGE=-0.06740 END !
ATOM H6' TYPE=HC CHARGE= 0.12560 END !
ATOM C8' TYPE=C8 CHARGE=-0.40430 END !
ATOM H8'1 TYPE=H8 CHARGE= 0.15500 END !
ATOM H8'2 TYPE=H8 CHARGE= 0.15500 END !
ATOM O3' TYPE=OS CHARGE=-0.57750 END !
BOND P O1P
```

BOND P O2P
BOND P O5'
BOND O5' C5'
BOND C5' C4'
BOND C5' C6'
BOND C5' C8'
BOND C4' H4'
BOND C4' O4'
BOND C4' C3'
BOND O4' C1'
BOND C1' H1'
BOND C1' N9
BOND C1' C2'
BOND N9 C8
BOND N9 C4
BOND C8 H8
BOND C8 N7
BOND N7 C5
BOND C5 C6
BOND C5 C4
BOND C6 N6
BOND C6 N1
BOND N6 H61
BOND N6 H62
BOND N1 C2
BOND C2 H2
BOND C2 N3
BOND N3 C4
BOND C3' C2'
BOND C3' O3'
BOND C3' C7'
BOND C2' H2'1
BOND C2' H2'2
BOND C7' H7'1
BOND C7' H7'2
BOND C7' C6'
BOND C6' H6'
BOND C6' C8'
BOND C8' H8'1
BOND C8' H8'2
IMPR C4 C8 N9 C1'
IMPR N9 N7 C8 H8
IMPR C5 N1 C6 N6
IMPR N1 N3 C2 H2
IMPR C6 H61 N6 H62
! IMPRoper to keep the two purine rings parallel:
IMPR C8 C4 C5 N1
IMPR N3 C4 C5 N7
IMPR C8 C5 C4 C2
IMPR C6 C5 C4 N9
! Other

IMPRoper N9 C4 C5 N7
IMPRoper C5 N7 C8 N9
IMPRoper C8 N9 C4 C5
IMPRoper C5 C6 N6 H61
END

RESI TT ! Tc-THYMINE

ATOM P TYPE=P CHARGE= 1.21660 END !
ATOM O1P TYPE=O2 CHARGE=-0.79140 END !
ATOM O2P TYPE=O2 CHARGE=-0.79140 END !
ATOM O5' TYPE=OS CHARGE=-0.49280 END !
ATOM C5' TYPE=C5 CHARGE= 0.20640 END !
ATOM C4' TYPE=CT CHARGE= 0.19590 END !
ATOM H4' TYPE=H1 CHARGE= 0.09370 END !
ATOM O4' TYPE=OS CHARGE=-0.45860 END !
ATOM C1' TYPE=CT CHARGE= 0.19280 END !
ATOM H1' TYPE=H2 CHARGE= 0.09620 END !
ATOM N1 TYPE=N* CHARGE= 0.00980 END !
ATOM C6 TYPE=CM CHARGE=-0.20290 END !
ATOM H6 TYPE=H4 CHARGE= 0.21610 END !
ATOM C5 TYPE=CM CHARGE=-0.01550 END !
ATOM C7 TYPE=CT CHARGE=-0.27030 END !
ATOM H71 TYPE=HC CHARGE= 0.09290 END !
ATOM H72 TYPE=HC CHARGE= 0.09290 END !
ATOM H73 TYPE=HC CHARGE= 0.09290 END !
ATOM C4 TYPE=C CHARGE= 0.53960 END !
ATOM O4 TYPE=O CHARGE=-0.54300 END !
ATOM N3 TYPE=NA CHARGE=-0.45100 END !
ATOM H3 TYPE=H CHARGE= 0.34060 END !
ATOM C2 TYPE=C CHARGE= 0.54240 END !
ATOM O2 TYPE=O CHARGE=-0.59320 END !
ATOM C3' TYPE=CT CHARGE= 0.27860 END !
ATOM C2' TYPE=CT CHARGE=-0.07600 END !
ATOM H2'1 TYPE=HC CHARGE= 0.05590 END !
ATOM H2'2 TYPE=HC CHARGE= 0.05590 END !
ATOM C7' TYPE=CT CHARGE=-0.10070 END !
ATOM H7'1 TYPE=HC CHARGE= 0.04060 END !
ATOM H7'2 TYPE=HC CHARGE= 0.04060 END !
ATOM C6' TYPE=C6 CHARGE=-0.06740 END !
ATOM H6' TYPE=HC CHARGE= 0.12560 END !
ATOM C8' TYPE=C8 CHARGE=-0.40430 END !
ATOM H8'1 TYPE=H8 CHARGE= 0.15500 END !
ATOM H8'2 TYPE=H8 CHARGE= 0.15500 END !
ATOM O3' TYPE=OS CHARGE=-0.57750 END !
BOND P O1P
BOND P O2P
BOND P O5'
BOND O5' C5'
BOND C5' C4'
BOND C5' C6'
BOND C5' C8'

BOND C4' H4'
 BOND C4' O4'
 BOND C4' C3'
 BOND O4' C1'
 BOND C1' H1'
 BOND C1' N1
 BOND C1' C2'
 BOND N1 C6
 BOND N1 C2
 BOND C6 H6
 BOND C6 C5
 BOND C5 C7
 BOND C5 C4
 BOND C7 H71
 BOND C7 H72
 BOND C7 H73
 BOND C4 O4
 BOND C4 N3
 BOND N3 H3
 BOND N3 C2
 BOND C2 O2
 BOND C3' C2'
 BOND C3' O3'
 BOND C3' C7'
 BOND C2' H2'1
 BOND C2' H2'2
 BOND C7' H7'1
 BOND C7' H7'2
 BOND C7' C6'
 BOND C6' H6'
 BOND C6' C8'
 BOND C8' H8'1
 BOND C8' H8'2
 IMPR C2 C6 N1 C1'
 IMPR C4 C6 C5 C7
 IMPR N1 N3 C2 O2
 IMPR C5 N3 C4 O4
 IMPR C4 C2 N3 H3
 IMPR N1 C5 C6 H6
 IMPR N1 C6 C5 C7
 !other
 IMPRoper C1' C2 C6 N1
 IMPRoper C4 C5 C6 N1
 IMPRoper N1 C2 N3 C4
 IMPRoper C6 N1 C2 N3
 END

RESI TG ! Tc-GUANINE

ATOM P TYPE=P CHARGE= 1.21660 END !
 ATOM O1P TYPE=O2 CHARGE=-0.79140 END !
 ATOM O2P TYPE=O2 CHARGE=-0.79140 END !

ATOM	O5'	TYPE=OS	CHARGE=-0.49280 END !
ATOM	C5'	TYPE=C5	CHARGE= 0.20640 END !
ATOM	C4'	TYPE=CT	CHARGE= 0.19590 END !
ATOM	H4'	TYPE=H1	CHARGE= 0.09370 END !
ATOM	O4'	TYPE=OS	CHARGE=-0.45860 END !
ATOM	C1'	TYPE=CT	CHARGE= 0.12510 END !
ATOM	H1'	TYPE=H2	CHARGE= 0.12920 END !
ATOM	N9	TYPE=N*	CHARGE= 0.00540 END !
ATOM	C8	TYPE=CK	CHARGE= 0.17740 END !
ATOM	H8	TYPE=H5	CHARGE= 0.15680 END !
ATOM	N7	TYPE=NB	CHARGE=-0.58030 END !
ATOM	C5	TYPE=CB	CHARGE= 0.14320 END !
ATOM	C6	TYPE=C	CHARGE= 0.55740 END !
ATOM	O6	TYPE=O	CHARGE=-0.54950 END !
ATOM	N1	TYPE=NA	CHARGE=-0.58840 END !
ATOM	H1	TYPE=H	CHARGE= 0.36700 END !
ATOM	C2	TYPE=CA	CHARGE= 0.79380 END !
ATOM	N2	TYPE=N2	CHARGE=-0.91350 END !
ATOM	H21	TYPE=H	CHARGE= 0.39740 END !
ATOM	H22	TYPE=H	CHARGE= 0.39740 END !
ATOM	N3	TYPE=NC	CHARGE=-0.68500 END !
ATOM	C4	TYPE=CB	CHARGE= 0.20690 END !
ATOM	C3'	TYPE=CT	CHARGE= 0.27860 END !
ATOM	C2'	TYPE=CT	CHARGE=-0.07600 END !
ATOM	H2'1	TYPE=HC	CHARGE= 0.05590 END !
ATOM	H2'2	TYPE=HC	CHARGE= 0.05590 END !
ATOM	C7'	TYPE=CT	CHARGE=-0.10070 END !
ATOM	H7'1	TYPE=HC	CHARGE= 0.04060 END !
ATOM	H7'2	TYPE=HC	CHARGE= 0.04060 END !
ATOM	C6'	TYPE=C6	CHARGE=-0.06740 END !
ATOM	H6'	TYPE=HC	CHARGE= 0.12560 END !
ATOM	C8'	TYPE=C8	CHARGE=-0.40430 END !
ATOM	H8'1	TYPE=H8	CHARGE= 0.15500 END !
ATOM	H8'2	TYPE=H8	CHARGE= 0.15500 END !
ATOM	O3'	TYPE=OS	CHARGE=-0.57750 END !
BOND	P	O1P	
BOND	P	O2P	
BOND	P	O5'	
BOND	O5'	C5'	
BOND	C5'	C4'	
BOND	C5'	C6'	
BOND	C5'	C8'	
BOND	C4'	H4'	
BOND	C4'	O4'	
BOND	C4'	C3'	
BOND	O4'	C1'	
BOND	C1'	H1'	
BOND	C1'	N9	
BOND	C1'	C2'	
BOND	N9	C8	
BOND	N9	C4	

BOND C8 H8
 BOND C8 N7
 BOND N7 C5
 BOND C5 C6
 BOND C5 C4
 BOND C6 O6
 BOND C6 N1
 BOND N1 H1
 BOND N1 C2
 BOND C2 N2
 BOND C2 N3
 BOND N2 H21
 BOND N2 H22
 BOND N3 C4
 BOND C3' C2'
 BOND C3' O3'
 BOND C3' C7'
 BOND C2' H2'1
 BOND C2' H2'2
 BOND C7' H7'1
 BOND C7' H7'2
 BOND C7' C6'
 BOND C6' H6'
 BOND C6' C8'
 BOND C8' H8'1
 BOND C8' H8'2
 IMPR C4 C8 N9 C1'
 IMPR C5 N1 C6 O6
 IMPR C6 C2 N1 H1
 IMPR C2 H21 N2 H22
 IMPR N9 N7 C8 H8
 IMPR N2 N1 C2 N3

!IMPRoper to keep the two purine rings parallel:

IMPR C8 C4 C5 N1
 IMPR C8 C5 C4 C2
 IMPR N3 C4 C5 N7
 IMPR C6 C5 C4 N9
 !other
 IMPRoper N3 C2 N2 H21
 IMPRoper N1 C2 N2 H22
 IMPRoper N3 C2 N1 H1
 IMPRoper N9 C4 C5 N7
 IMPRoper C5 N7 C8 N9
 IMPRoper C8 N9 C4 C5
 END

RESI TG5 ! Tc-GUANINE 5' terminal

ATOM H5T TYPE=HO CHARGE= 0.42470 END !
 ATOM O5' TYPE=OH CHARGE= -0.60250 END !

ATOM	C5'	TYPE=C5	CHARGE= 0.20640 END !
ATOM	C4'	TYPE=CT	CHARGE= 0.19590 END !
ATOM	H4'	TYPE=H1	CHARGE= 0.09370 END !
ATOM	O4'	TYPE=OS	CHARGE=-0.45860 END !
ATOM	C1'	TYPE=CT	CHARGE= 0.12510 END !
ATOM	H1'	TYPE=H2	CHARGE= 0.12920 END !
ATOM	N9	TYPE=N*	CHARGE= 0.00540 END !
ATOM	C8	TYPE=CK	CHARGE= 0.17740 END !
ATOM	H8	TYPE=H5	CHARGE= 0.15680 END !
ATOM	N7	TYPE=NB	CHARGE=-0.58030 END !
ATOM	C5	TYPE=CB	CHARGE= 0.14320 END !
ATOM	C6	TYPE=C	CHARGE= 0.55740 END !
ATOM	O6	TYPE=O	CHARGE=-0.54950 END !
ATOM	N1	TYPE=NA	CHARGE=-0.58840 END !
ATOM	H1	TYPE=H	CHARGE= 0.36700 END !
ATOM	C2	TYPE=CA	CHARGE= 0.79380 END !
ATOM	N2	TYPE=N2	CHARGE=-0.91350 END !
ATOM	H21	TYPE=H	CHARGE= 0.39740 END !
ATOM	H22	TYPE=H	CHARGE= 0.39740 END !
ATOM	N3	TYPE=NC	CHARGE=-0.68500 END !
ATOM	C4	TYPE=CB	CHARGE= 0.20690 END !
ATOM	C3'	TYPE=CT	CHARGE= 0.27860 END !
ATOM	C2'	TYPE=CT	CHARGE=-0.07600 END !
ATOM	H2'1	TYPE=HC	CHARGE= 0.05590 END !
ATOM	H2'2	TYPE=HC	CHARGE= 0.05590 END !
ATOM	C7'	TYPE=CT	CHARGE=-0.10070 END !
ATOM	H7'1	TYPE=HC	CHARGE= 0.04060 END !
ATOM	H7'2	TYPE=HC	CHARGE= 0.04060 END !
ATOM	C6'	TYPE=C6	CHARGE=-0.06740 END !
ATOM	H6'	TYPE=HC	CHARGE= 0.12560 END !
ATOM	C8'	TYPE=C8	CHARGE=-0.40430 END !
ATOM	H8'1	TYPE=H8	CHARGE= 0.15500 END !
ATOM	H8'2	TYPE=H8	CHARGE= 0.15500 END !
ATOM	O3'	TYPE=OS	CHARGE=-0.57750 END !
BOND	H5T	O5'	
BOND	O5'	C5'	
BOND	C5'	C4'	
BOND	C5'	C6'	
BOND	C5'	C8'	
BOND	C4'	H4'	
BOND	C4'	O4'	
BOND	C4'	C3'	
BOND	O4'	C1'	
BOND	C1'	H1'	
BOND	C1'	N9	
BOND	C1'	C2'	
BOND	N9	C8	
BOND	N9	C4	
BOND	C8	H8	
BOND	C8	N7	
BOND	N7	C5	

BOND C5 C6
 BOND C5 C4
 BOND C6 O6
 BOND C6 N1
 BOND N1 H1
 BOND N1 C2
 BOND C2 N2
 BOND C2 N3
 BOND N2 H21
 BOND N2 H22
 BOND N3 C4
 BOND C3' C2'
 BOND C3' O3'
 BOND C3' C7'
 BOND C2' H2'1
 BOND C2' H2'2
 BOND C7' H7'1
 BOND C7' H7'2
 BOND C7' C6'
 BOND C6' H6'
 BOND C6' C8'
 BOND C8' H8'1
 BOND C8' H8'2
 IMPR C4 C8 N9 C1'
 IMPR C5 N1 C6 O6
 IMPR C6 C2 N1 H1
 IMPR C2 H21 N2 H22
 IMPR N9 N7 C8 H8
 IMPR N2 N1 C2 N3

!IMPRoper to keep the two purine rings parallel:

IMPR C8 C4 C5 N1
 IMPR C8 C5 C4 C2
 IMPR N3 C4 C5 N7
 IMPR C6 C5 C4 N9
 !other
 IMPRoper N3 C2 N2 H21
 IMPRoper N1 C2 N2 H22
 IMPRoper N3 C2 N1 H1
 IMPRoper N9 C4 C5 N7
 IMPRoper C5 N7 C8 N9
 IMPRoper C8 N9 C4 C5
 END

RESI TG3 ! Tc-GUANINE

ATOM P TYPE=P CHARGE= 1.21660 END !
 ATOM O1P TYPE=O2 CHARGE=-0.79140 END !
 ATOM O2P TYPE=O2 CHARGE=-0.79140 END !
 ATOM O5' TYPE=OS CHARGE=-0.49280 END !
 ATOM C5' TYPE=C5 CHARGE= 0.20640 END !
 ATOM C4' TYPE=CT CHARGE= 0.19590 END !

ATOM	H4'	TYPE=H1	CHARGE= 0.09370 END !
ATOM	O4'	TYPE=OS	CHARGE=-0.45860 END !
ATOM	C1'	TYPE=CT	CHARGE= 0.12510 END !
ATOM	H1'	TYPE=H2	CHARGE= 0.12920 END !
ATOM	N9	TYPE=N*	CHARGE= 0.00540 END !
ATOM	C8	TYPE=CK	CHARGE= 0.17740 END !
ATOM	H8	TYPE=H5	CHARGE= 0.15680 END !
ATOM	N7	TYPE=NB	CHARGE=-0.58030 END !
ATOM	C5	TYPE=CB	CHARGE= 0.14320 END !
ATOM	C6	TYPE=C	CHARGE= 0.55740 END !
ATOM	O6	TYPE=O	CHARGE=-0.54950 END !
ATOM	N1	TYPE=NA	CHARGE=-0.58840 END !
ATOM	H1	TYPE=H	CHARGE= 0.36700 END !
ATOM	C2	TYPE=CA	CHARGE= 0.79380 END !
ATOM	N2	TYPE=N2	CHARGE=-0.91350 END !
ATOM	H21	TYPE=H	CHARGE= 0.39740 END !
ATOM	H22	TYPE=H	CHARGE= 0.39740 END !
ATOM	N3	TYPE=NC	CHARGE=-0.68500 END !
ATOM	C4	TYPE=CB	CHARGE= 0.20690 END !
ATOM	C3'	TYPE=CT	CHARGE= 0.27860 END !
ATOM	C2'	TYPE=CT	CHARGE=-0.07600 END !
ATOM	H2'1	TYPE=HC	CHARGE= 0.05590 END !
ATOM	H2'2	TYPE=HC	CHARGE= 0.05590 END !
ATOM	C7'	TYPE=CT	CHARGE=-0.10070 END !
ATOM	H7'1	TYPE=HC	CHARGE= 0.04060 END !
ATOM	H7'2	TYPE=HC	CHARGE= 0.04060 END !
ATOM	C6'	TYPE=C6	CHARGE=-0.06740 END !
ATOM	H6'	TYPE=HC	CHARGE= 0.12560 END !
ATOM	C8'	TYPE=C8	CHARGE=-0.40430 END !
ATOM	H8'1	TYPE=H8	CHARGE= 0.15500 END !
ATOM	H8'2	TYPE=H8	CHARGE= 0.15500 END !
ATOM	O3'	TYPE=OH	CHARGE= -0.57750 END !
ATOM	H3T	TYPE=HO	CHARGE= 0.44190 END !
BOND	P	O1P	
BOND	P	O2P	
BOND	P	O5'	
BOND	O5'	C5'	
BOND	C5'	C4'	
BOND	C5'	C6'	
BOND	C5'	C8'	
BOND	C4'	H4'	
BOND	C4'	O4'	
BOND	C4'	C3'	
BOND	O4'	C1'	
BOND	C1'	H1'	
BOND	C1'	N9	
BOND	C1'	C2'	
BOND	N9	C8	
BOND	N9	C4	
BOND	C8	H8	
BOND	C8	N7	

BOND N7 C5
 BOND C5 C6
 BOND C5 C4
 BOND C6 O6
 BOND C6 N1
 BOND N1 H1
 BOND N1 C2
 BOND C2 N2
 BOND C2 N3
 BOND N2 H21
 BOND N2 H22
 BOND N3 C4
 BOND C3' C2'
 BOND C3' O3'
 BOND C3' C7'
 BOND C2' H2'1
 BOND C2' H2'2
 BOND C7' H7'1
 BOND C7' H7'2
 BOND C7' C6'
 BOND C6' H6'
 BOND C6' C8'
 BOND C8' H8'1
 BOND C8' H8'2
 BOND O3' H3T
 IMPR C4 C8 N9 C1'
 IMPR C5 N1 C6 O6
 IMPR C6 C2 N1 H1
 IMPR C2 H21 N2 H22
 IMPR N9 N7 C8 H8
 IMPR N2 N1 C2 N3
 !IMPRoper to keep the two purine rings parallel:
 IMPR C8 C4 C5 N1
 IMPR C8 C5 C4 C2
 IMPR N3 C4 C5 N7
 IMPR C6 C5 C4 N9
 !other
 IMPRoper N3 C2 N2 H21
 IMPRoper N1 C2 N2 H22
 IMPRoper N3 C2 N1 H1
 IMPRoper N9 C4 C5 N7
 IMPRoper C5 N7 C8 N9
 IMPRoper C8 N9 C4 C5
 END

RESI TC ! Tc-CYTOSINE

ATOM P TYPE=P CHARGE= 1.16590 END !
 ATOM O1P TYPE=O2 CHARGE=-0.77610 END !
 ATOM O2P TYPE=O2 CHARGE=-0.77610 END !
 ATOM O5' TYPE=OS CHARGE=-0.49280 END !

ATOM	C5'	TYPE=C5	CHARGE= 0.19720 END !
ATOM	C4'	TYPE=CT	CHARGE= 0.17180 END !
ATOM	H4'	TYPE=H1	CHARGE= 0.09000 END !
ATOM	O4'	TYPE=OS	CHARGE=-0.43510 END !
ATOM	C1'	TYPE=CT	CHARGE= 0.17170 END !
ATOM	H1'	TYPE=H2	CHARGE= 0.11130 END !
ATOM	N1	TYPE=N*	CHARGE=-0.03390 END !
ATOM	C6	TYPE=CM	CHARGE=-0.01830 END !
ATOM	H6	TYPE=H4	CHARGE= 0.22930 END !
ATOM	C5	TYPE=CM	CHARGE=-0.52220 END !
ATOM	H5	TYPE=HA	CHARGE= 0.18630 END !
ATOM	C4	TYPE=CA	CHARGE= 0.84390 END !
ATOM	N4	TYPE=N2	CHARGE=-0.97730 END !
ATOM	H41	TYPE=H	CHARGE= 0.43140 END !
ATOM	H42	TYPE=H	CHARGE= 0.43140 END !
ATOM	N3	TYPE=NC	CHARGE=-0.77480 END !
ATOM	C2	TYPE=C	CHARGE= 0.79590 END !
ATOM	O2	TYPE=O	CHARGE=-0.65480 END !
ATOM	C3'	TYPE=CT	CHARGE= 0.31340 END !
ATOM	C2'	TYPE=CT	CHARGE=-0.12520 END !
ATOM	H2'1	TYPE=HC	CHARGE= 0.06110 END !
ATOM	H2'2	TYPE=HC	CHARGE= 0.06110 END !
ATOM	C7'	TYPE=CT	CHARGE=-0.13230 END !
ATOM	H7'1	TYPE=HC	CHARGE= 0.04620 END !
ATOM	H7'2	TYPE=HC	CHARGE= 0.04620 END !
ATOM	C6'	TYPE=C6	CHARGE=-0.04910 END !
ATOM	H6'	TYPE=HC	CHARGE= 0.11380 END !
ATOM	C8'	TYPE=C8	CHARGE=-0.35080 END !
ATOM	H8'1	TYPE=H8	CHARGE= 0.13530 END !
ATOM	H8'2	TYPE=H8	CHARGE= 0.13530 END !
ATOM	O3'	TYPE=OS	CHARGE=-0.57750 END !
BOND	P	O1P	
BOND	P	O2P	
BOND	P	O5'	
BOND	O5'	C5'	
BOND	C5'	C4'	
BOND	C5'	C6'	
BOND	C5'	C8'	
BOND	C4'	H4'	
BOND	C4'	O4'	
BOND	C4'	C3'	
BOND	O4'	C1'	
BOND	C1'	H1'	
BOND	C1'	N1	
BOND	C1'	C2'	
BOND	N1	C6	
BOND	N1	C2	
BOND	C6	H6	
BOND	C6	C5	
BOND	C5	H5	
BOND	C5	C4	

BOND C4 N4
 BOND C4 N3
 BOND N4 H41
 BOND N4 H42
 BOND N3 C2
 BOND C2 O2
 BOND C3' C2'
 BOND C3' O3'
 BOND C3' C7'
 BOND C2' H2'1
 BOND C2' H2'2
 BOND C7' H7'1
 BOND C7' H7'2
 BOND C7' C6'
 BOND C6' H6'
 BOND C6' C8'
 BOND C8' H8'1
 BOND C8' H8'2
 IMPR C2 C6 N1 C1'
 IMPR N1 N3 C2 O2
 IMPR C4 H41 N4 H42
 IMPR N1 C5 C6 H6
 IMPR C6 C4 C5 H5
 IMPR C5 N4 C4 N3
 !Other
 IMPRoper C5 C4 N4 H41
 IMPRoper C5 C6 N1 C2
 IMPRoper N3 C4 C5 C6
 IMPRoper C2 N3 C4 C5
 END

RESI TM ! Tc-MetCYT

ATOM	P	TYPE=P	CHARGE= 1.21660 END !
ATOM	O1P	TYPE=O2	CHARGE= -0.79140 END !
ATOM	O2P	TYPE=O2	CHARGE= -0.79140 END !
ATOM	O5'	TYPE=OS	CHARGE= -0.49280 END !
ATOM	C5'	TYPE=C5	CHARGE= 0.20640 END !
ATOM	C4'	TYPE=CT	CHARGE= 0.19590 END !
ATOM	H4'	TYPE=H1	CHARGE= 0.09370 END !
ATOM	O4'	TYPE=OS	CHARGE= -0.45860 END !
ATOM	C1'	TYPE=CT	CHARGE= 0.12510 END !
ATOM	H1'	TYPE=H2	CHARGE= 0.12920 END !
ATOM	N1	TYPE=N*	CHARGE= -0.04560 END !
ATOM	C6	TYPE=CM	CHARGE= -0.11830 END !
ATOM	H6	TYPE=H4	CHARGE= 0.19310 END !
ATOM	C5	TYPE=CM	CHARGE= -0.10920 END !
ATOM	C7	TYPE=CT	CHARGE= -0.20040 END !
ATOM	H71	TYPE=HC	CHARGE= 0.06980 END !
ATOM	H72	TYPE=HC	CHARGE= 0.06980 END !
ATOM	H73	TYPE=HC	CHARGE= 0.06980 END !
ATOM	C4	TYPE=CA	CHARGE= 0.61570 END !

ATOM N4 TYPE=N2 CHARGE= -0.85710 END !
ATOM H41 TYPE=H CHARGE= 0.39440 END !
ATOM H42 TYPE=H CHARGE= 0.39440 END !
ATOM N3 TYPE=NC CHARGE= -0.72040 END !
ATOM C2 TYPE=C CHARGE= 0.78250 END !
ATOM O2 TYPE=O CHARGE= -0.65370 END !
ATOM C3' TYPE=CT CHARGE= 0.27860 END !
ATOM C2' TYPE=CT CHARGE= -0.07600 END !
ATOM H2'1 TYPE=HC CHARGE= 0.05590 END !
ATOM H2'2 TYPE=HC CHARGE= 0.05590 END !
ATOM C7' TYPE=CT CHARGE= -0.10070 END !
ATOM H7'1 TYPE=HC CHARGE= 0.04060 END !
ATOM H7'2 TYPE=HC CHARGE= 0.04060 END !
ATOM C6' TYPE=C6 CHARGE= -0.06740 END !
ATOM H6' TYPE=HC CHARGE= 0.12560 END !
ATOM C8' TYPE=C8 CHARGE= -0.40430 END !
ATOM H8'1 TYPE=H8 CHARGE= 0.15500 END !
ATOM H8'2 TYPE=H8 CHARGE= 0.15500 END !
ATOM O3' TYPE=OS CHARGE= -0.57750 END !
BOND P O1P
BOND P O2P
BOND P O5'
BOND O5' C5'
BOND C5' C4'
BOND C5' C6'
BOND C5' C8'
BOND C4' H4'
BOND C4' O4'
BOND C4' C3'
BOND O4' C1'
BOND C1' H1'
BOND C1' N1
BOND C1' C2'
BOND N1 C6
BOND N1 C2
BOND C6 H6
BOND C6 C5
BOND C5 C7
BOND C7 H71
BOND C7 H72
BOND C7 H73
BOND C5 C4
BOND C4 N4
BOND C4 N3
BOND N4 H41
BOND N4 H42
BOND N3 C2
BOND C2 O2
BOND C3' C2'
BOND C3' O3'
BOND C3' C7'

BOND C2' H2'1
 BOND C2' H2'2
 BOND C7' H7'1
 BOND C7' H7'2
 BOND C7' C6'
 BOND C6' H6'
 BOND C6' C8'
 BOND C8' H8'1
 BOND C8' H8'2
 IMPR C2 C6 N1 C1'
 IMPR N1 N3 C2 O2
 IMPR C4 H41 N4 H42
 IMPR N1 C5 C6 H6
 IMPR C4 C6 C5 C7
 IMPR C5 N4 C4 N3
 IMPR N1 C6 C5 C7
 !Other
 IMPRoper C5 C4 N4 H41
 IMPRoper N3 C4 N4 H42
 IMPRoper C5 C6 N1 C2
 IMPRoper N3 C4 C5 C6
 IMPRoper C2 N3 C4 C5
 END

RESI TM5 ! Tc-MetCYT 5'terminal

ATOM H5T TYPE=HO CHARGE= 0.42470 END !
 ATOM O5' TYPE=OH CHARGE= -0.60250 END !
 ATOM C5' TYPE=C5 CHARGE= 0.20640 END !
 ATOM C4' TYPE=CT CHARGE= 0.19590 END !
 ATOM H4' TYPE=H1 CHARGE= 0.09370 END !
 ATOM O4' TYPE=OS CHARGE= -0.45860 END !
 ATOM C1' TYPE=CT CHARGE= 0.12510 END !
 ATOM H1' TYPE=H2 CHARGE= 0.12920 END !
 ATOM N1 TYPE=N* CHARGE= -0.04560 END !
 ATOM C6 TYPE=CM CHARGE= -0.11830 END !
 ATOM H6 TYPE=H4 CHARGE= 0.19310 END !
 ATOM C5 TYPE=CM CHARGE= -0.10920 END !
 ATOM C7 TYPE=CT CHARGE= -0.20040 END !
 ATOM H71 TYPE=HC CHARGE= 0.06980 END !
 ATOM H72 TYPE=HC CHARGE= 0.06980 END !
 ATOM H73 TYPE=HC CHARGE= 0.06980 END !
 ATOM C4 TYPE=CA CHARGE= 0.61570 END !
 ATOM N4 TYPE=N2 CHARGE= -0.85710 END !
 ATOM H41 TYPE=H CHARGE= 0.39440 END !
 ATOM H42 TYPE=H CHARGE= 0.39440 END !
 ATOM N3 TYPE=NC CHARGE= -0.72040 END !
 ATOM C2 TYPE=C CHARGE= 0.78250 END !
 ATOM O2 TYPE=O CHARGE= -0.65370 END !
 ATOM C3' TYPE=CT CHARGE= 0.27860 END !
 ATOM C2' TYPE=CT CHARGE= -0.07600 END !
 ATOM H2'1 TYPE=HC CHARGE= 0.05590 END !

ATOM H2'2 TYPE=HC CHARGE= 0.05590 END !
ATOM C7' TYPE=CT CHARGE= -0.10070 END !
ATOM H7'1 TYPE=HC CHARGE= 0.04060 END !
ATOM H7'2 TYPE=HC CHARGE= 0.04060 END !
ATOM C6' TYPE=C6 CHARGE= -0.06740 END !
ATOM H6' TYPE=HC CHARGE= 0.12560 END !
ATOM C8' TYPE=C8 CHARGE= -0.40430 END !
ATOM H8'1 TYPE=H8 CHARGE= 0.15500 END !
ATOM H8'2 TYPE=H8 CHARGE= 0.15500 END !
ATOM O3' TYPE=OS CHARGE= -0.57750 END !
BOND H5T O5'
BOND O5' C5'
BOND C5' C4'
BOND C5' C6'
BOND C5' C8'
BOND C4' H4'
BOND C4' O4'
BOND C4' C3'
BOND O4' C1'
BOND C1' H1'
BOND C1' N1
BOND C1' C2'
BOND N1 C6
BOND N1 C2
BOND C6 H6
BOND C6 C5
BOND C5 C7
BOND C7 H71
BOND C7 H72
BOND C7 H73
BOND C5 C4
BOND C4 N4
BOND C4 N3
BOND N4 H41
BOND N4 H42
BOND N3 C2
BOND C2 O2
BOND C3' C2'
BOND C3' O3'
BOND C3' C7'
BOND C2' H2'1
BOND C2' H2'2
BOND C7' H7'1
BOND C7' H7'2
BOND C7' C6'
BOND C6' H6'
BOND C6' C8'
BOND C8' H8'1
BOND C8' H8'2
IMPR C2 C6 N1 C1'
IMPR N1 N3 C2 O2

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IMPR C4 H41 N4 H42
IMPR N1 C5 C6 H6
IMPR C4 C6 C5 C7
IMPR C5 N4 C4 N3
IMPR N1 C6 C5 C7
!Other
IMPRoper C5 C4 N4 H41
IMPRoper N3 C4 N4 H42
IMPRoper C5 C6 N1 C2
IMPRoper N3 C4 C5 C6
IMPRoper C2 N3 C4 C5
END

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RESI TM3 ! Tc-MetCYT 3' terminal

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ATOM P TYPE=P CHARGE= 1.21660 END !
ATOM O1P TYPE=O2 CHARGE= -0.79140 END !
ATOM O2P TYPE=O2 CHARGE= -0.79140 END !
ATOM O5' TYPE=OS CHARGE= -0.49280 END !
ATOM C5' TYPE=C5 CHARGE= 0.20640 END !
ATOM C4' TYPE=CT CHARGE= 0.19590 END !
ATOM H4' TYPE=H1 CHARGE= 0.09370 END !
ATOM O4' TYPE=OS CHARGE= -0.45860 END !
ATOM C1' TYPE=CT CHARGE= 0.12510 END !
ATOM H1' TYPE=H2 CHARGE= 0.12920 END !
ATOM N1 TYPE=N* CHARGE= -0.04560 END !
ATOM C6 TYPE=CM CHARGE= -0.11830 END !
ATOM H6 TYPE=H4 CHARGE= 0.19310 END !
ATOM C5 TYPE=CM CHARGE= -0.10920 END !
ATOM C7 TYPE=CT CHARGE= -0.20040 END !
ATOM H71 TYPE=HC CHARGE= 0.06980 END !
ATOM H72 TYPE=HC CHARGE= 0.06980 END !
ATOM H73 TYPE=HC CHARGE= 0.06980 END !
ATOM C4 TYPE=CA CHARGE= 0.61570 END !
ATOM N4 TYPE=N2 CHARGE= -0.85710 END !
ATOM H41 TYPE=H CHARGE= 0.39440 END !
ATOM H42 TYPE=H CHARGE= 0.39440 END !
ATOM N3 TYPE=NC CHARGE= -0.72040 END !
ATOM C2 TYPE=C CHARGE= 0.78250 END !
ATOM O2 TYPE=O CHARGE= -0.65370 END !
ATOM C3' TYPE=CT CHARGE= 0.27860 END !
ATOM C2' TYPE=CT CHARGE= -0.07600 END !
ATOM H2'1 TYPE=HC CHARGE= 0.05590 END !
ATOM H2'2 TYPE=HC CHARGE= 0.05590 END !
ATOM C7' TYPE=CT CHARGE= -0.10070 END !
ATOM H7'1 TYPE=HC CHARGE= 0.04060 END !
ATOM H7'2 TYPE=HC CHARGE= 0.04060 END !
ATOM C6' TYPE=C6 CHARGE= -0.06740 END !
ATOM H6' TYPE=HC CHARGE= 0.12560 END !
ATOM C8' TYPE=C8 CHARGE= -0.40430 END !

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ATOM H8'1 TYPE=H8 CHARGE= 0.15500 END !
ATOM H8'2 TYPE=H8 CHARGE= 0.15500 END !
ATOM O3' TYPE=OH CHARGE= -0.57750 END !
ATOM H3T TYPE=HO CHARGE= 0.44190 END !
BOND P O1P
BOND P O2P
BOND P O5'
BOND O5' C5'
BOND C5' C4'
BOND C5' C6'
BOND C5' C8'
BOND C4' H4'
BOND C4' O4'
BOND C4' C3'
BOND O4' C1'
BOND C1' H1'
BOND C1' N1
BOND C1' C2'
BOND N1 C6
BOND N1 C2
BOND C6 H6
BOND C6 C5
BOND C5 C7
BOND C7 H71
BOND C7 H72
BOND C7 H73
BOND C5 C4
BOND C4 N4
BOND C4 N3
BOND N4 H41
BOND N4 H42
BOND N3 C2
BOND C2 O2
BOND C3' C2'
BOND C3' O3'
BOND C3' C7'
BOND C2' H2'1
BOND C2' H2'2
BOND C7' H7'1
BOND C7' H7'2
BOND C7' C6'
BOND C6' H6'
BOND C6' C8'
BOND C8' H8'1
BOND C8' H8'2
BOND O3' H3T
IMPR C2 C6 N1 C1'
IMPR N1 N3 C2 O2
IMPR C4 H41 N4 H42
IMPR N1 C5 C6 H6
IMPR C4 C6 C5 C7

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IMPR C5 N4 C4 N3
IMPR N1 C6 C5 C7
!Other
IMPRoper C5 C4 N4 H41
IMPRoper N3 C4 N4 H42
IMPRoper C5 C6 N1 C2
IMPRoper N3 C4 C5 C6
IMPRoper C2 N3 C4 C5
END

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BOND C6 CT 310.0 1.516 ! Kr same as CT-CT, bond length QM
BOND C6 C8 310.0 1.497 ! Kr same as CT-CT, bond length QM
BOND C6 C5 310.0 1.497 ! Kr same as CT-CT, bond length QM
BOND C5 C8 310.0 1.497 ! Kr same as CT-CT, bond length QM
BOND C5 OS 320.0 1.410 ! Kr same as CT-OS, bond length QM
BOND C5 OH 320.0 1.410 ! Kr same as CT-OH, bond length QM
BOND C5 CT 310.0 1.516 ! Kr same as CT-CT, bond length QM
BOND CT C8 310.0 1.526 ! Kr same as CT-CT, bond length QM
BOND C8 H8 340.0 1.090 ! same as CT-HC
BOND C6 HC 340.0 1.090 ! same as CT-HC
BOND C5 HC 340.0 1.090 ! same as CT-HC

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ANGL C8 C5 C6 160.0 60.00 ! K0 same as CT-CT-CT, angle QM
ANGL C5 C8 C6 160.0 60.00 ! K0 same as CT-CT-CT, angle QM
ANGL C8 C6 C5 160.0 60.00 ! K0 same as CT-CT-CT, angle QM
ANGL C6 C5 CT 150.0 109.50 ! K0 same as CT-CT-CT, angle QM
ANGL C6 CT CT 150.0 109.50 ! K0 same as CT-CT-CT, angle QM
ANGL C5 CT CT 150.0 109.50 ! K0 same as CT-CT-CT, angle QM
ANGL C5 C6 CT 150.0 109.50 ! K0 same as CT-CT-CT, angle QM
ANGL C6 C5 OS 150.0 119.50 ! K0 same as CT-CT-OS, angle QM
ANGL C8 C5 OS 150.0 119.50 ! K0 same as CT-CT-OS, angle QM
ANGL C5 CT OS 150.0 109.50 ! K0 same as CT-CT-OS angle QM
ANGL OS C5 CT 150.0 119.50 ! K0 same as CT-CT-OS, angle QM
ANGL C8 C5 CT 150.0 116.50 ! K0 same as CT-CT-CT, angle QM
ANGL C8 C6 CT 150.0 116.50 ! K0 same as CT-CT-CT, angle QM
ANGL H8 C8 H8 150.0 115.20 ! K0 same as HC-CT-HC, angle QM
ANGL C5 C8 H8 160.0 115.80 ! K0 same as CT-CT-HC, angle QM
ANGL C6 C8 H8 160.0 117.70 ! K0 same as CT-CT-HC, angle QM
ANGL C5 C6 HC 160.0 119.50 ! K0 same as CT-CT-HC, angle QM
ANGL C8 C6 HC 160.0 119.50 ! K0 same as CT-CT-HC, angle QM
ANGL CT C6 HC 160.0 119.70 ! K0 same as CT-CT-HC, angle QM
ANGL HC CT C6 160.0 109.50 ! K0 same as CT-CT-HC, angle QM

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