Electronic Supplementary Material (ESI) for Molecular BioSystems.

Supporting Information-Part III

How RNase HI (*Escherichia coli*) promoted site-selective hydrolysis works on RNA in duplex with carba-LNA and LNA substituted antisense strands in antisense strategy context

Oleksandr Plashkevych*, Qing Li, and Jyoti Chattopadhyaya*

Chemical Biology Program, Department of Cell and Molecular Biology, Box 581,
Biomedical Center, Uppsala University, SE-751 23 Uppsala, Sweden

*Corresponding Authors: Chemical Biology Program, Department of Cell and Molecular Biology. Biomedical Centre, Uppsala University, SE-75123 Uppsala, Sweden.
Phone: +46-18-4714577, Fax: +46-18-554495, Email: jyoti@boc.uu.se, oleksandr@boc.uu.se

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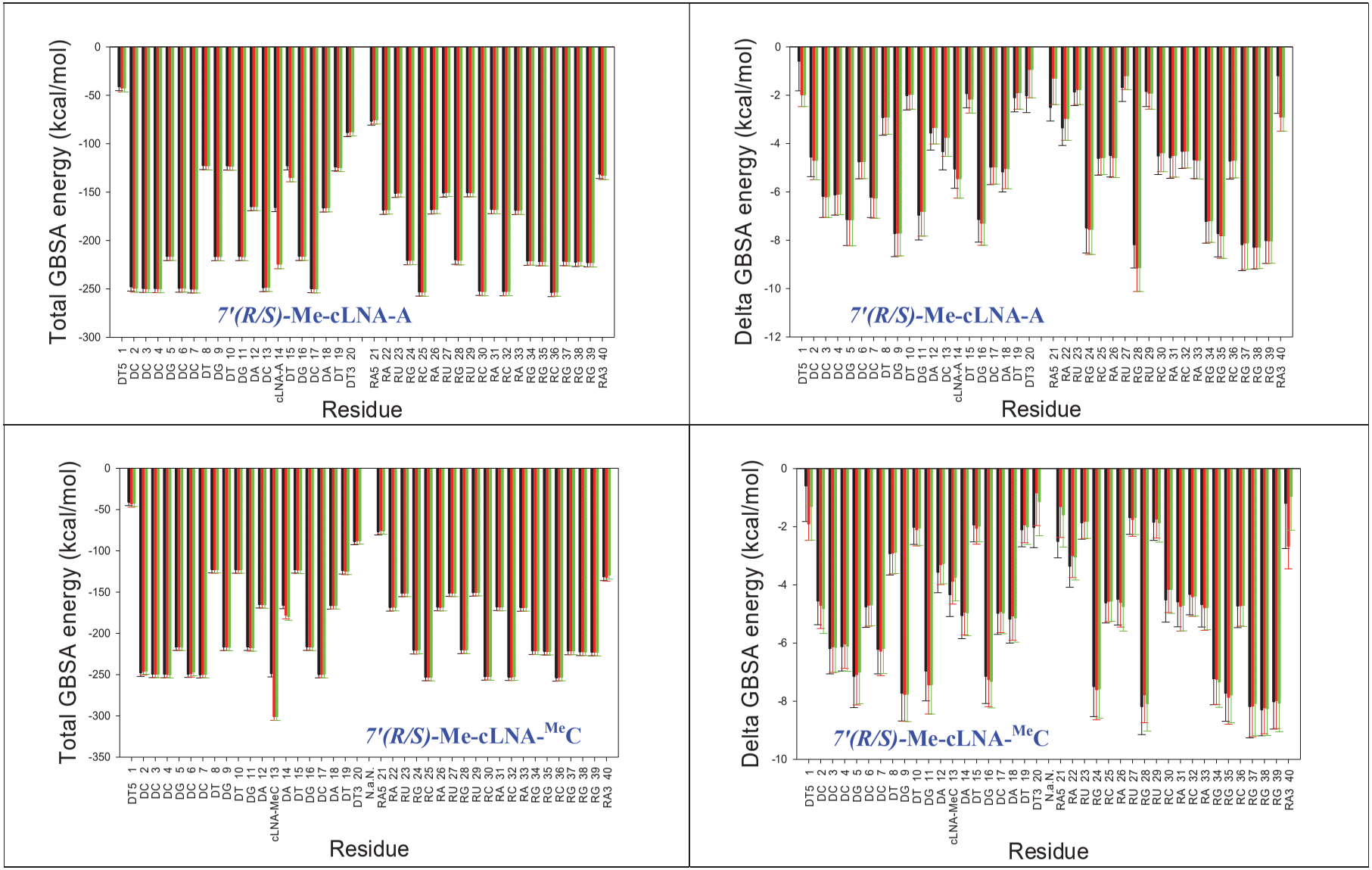
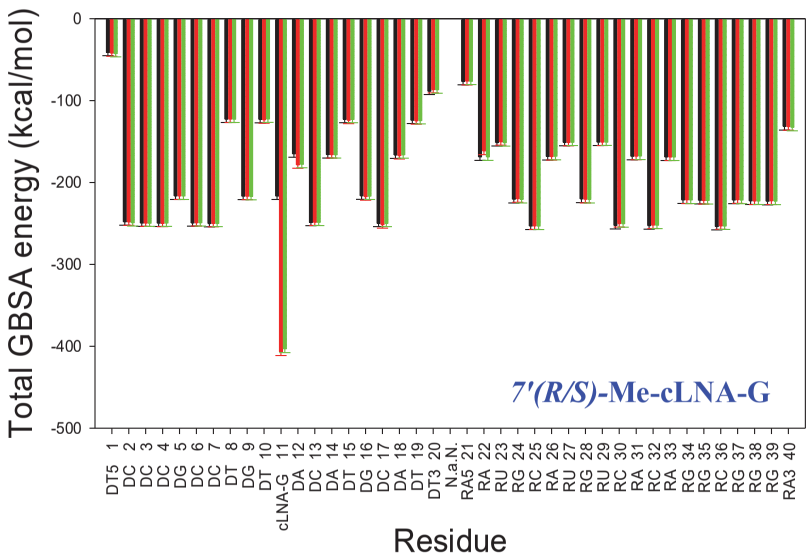
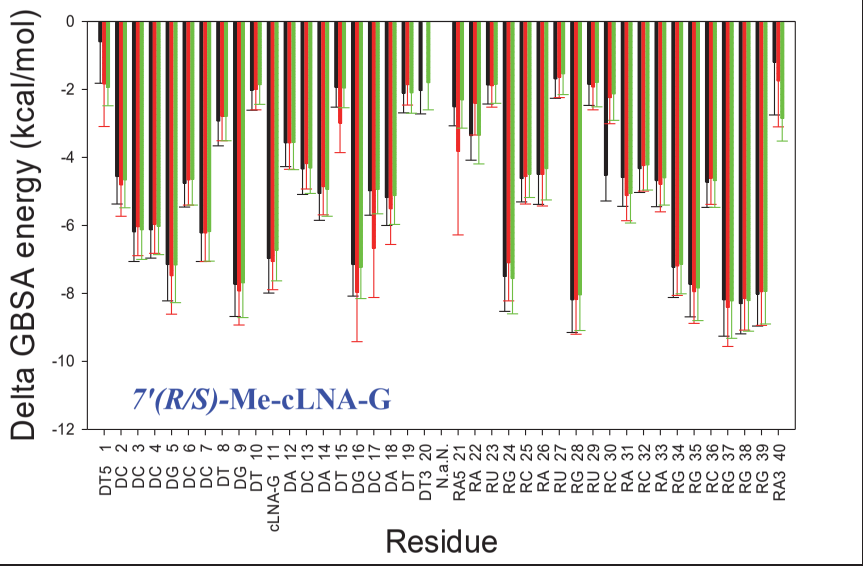
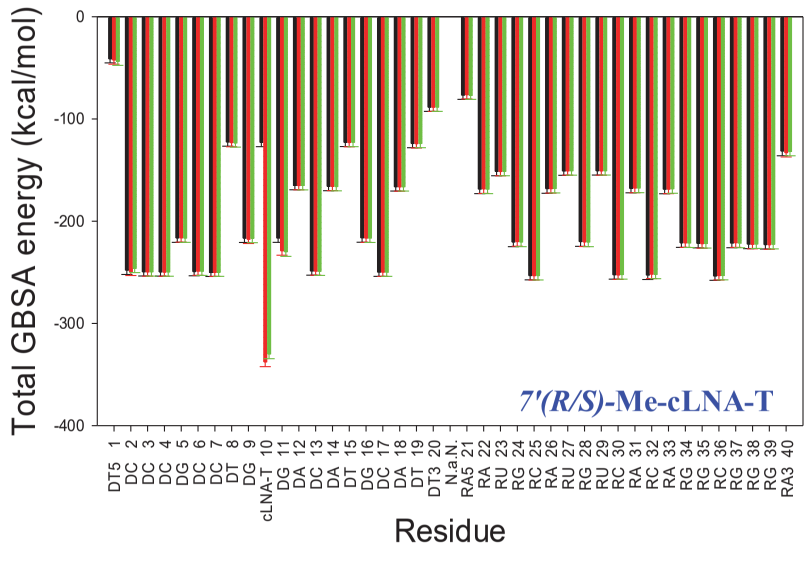
Figure SIII.1. Pair-wise comparison of the GBSA total energies (left column) and corresponding delta total GBSA energies (total energy of the duplex minus total energies of the individual strands), right column) along the MD trajectories of the *7'R*- and *7'S*-Me-cLNA modified duplexes in comparison with that of the native counterpart.




Total GBSA energy (kcal/mol)
0
-100
-200
-300
-400
-500
7′(R/S)-Me-cLNA-G
DT5 1 DC 2 DC 3 DC 4 DG 5 DC 6 DC 7 DT 8 DG 9 DT 10 cLNA-G 11 DA 12 DC 13 DA 14 DT 15 DG 16 DC 17 DA 18 DT 19 DT3 20 N.a.N. RA5 21 RA 22 RU 23 RG 24 RC 25 RA 26 RU 27 RG 28 RU 29 RC 30 RA 31 RC 32 RA 33 RG 34 RG 35 RC 36 RG 37 RG 38 RG 39 RA3 40
Residue


Delta GBSA energy (kcal/mol)
0
-2
-4
-6
-8
-10
-12
7′(R/S)-Me-cLNA-G
DT5 1 DC 2 DC 3 DC 4 DG 5 DC 6 DC 7 DT 8 DG 9 DT 10 cLNA-G 11 DA 12 DC 13 DA 14 DT 15 DG 16 DC 17 DA 18 DT 19 DT3 20 N.a.N. RA5 21 RA 22 RU 23 RG 24 RC 25 RA 26 RU 27 RG 28 RU 29 RC 30 RA 31 RC 32 RA 33 RG 34 RG 35 RC 36 RG 37 RG 38 RG 39 RA3 40
Residue


Total GBSA energy (kcal/mol)
0
-100
-200
-300
-400
7′(R/S)-Me-cLNA-T
DT5 1 DC 2 DC 3 DC 4 DG 5 DC 6 DC 7 DT 8 DG 9 cLNA-T 10 DG 11 DA 12 DC 13 DA 14 DT 15 DG 16 DC 17 DA 18 DT 19 DT3 20 N.a.N. RA5 21 RA 22 RU 23 RG 24 RC 25 RA 26 RU 27 RG 28 RU 29 RC 30 RA 31 RC 32 RA 33 RG 34 RG 35 RC 36 RG 37 RG 38 RG 39 RA3 40
Residue

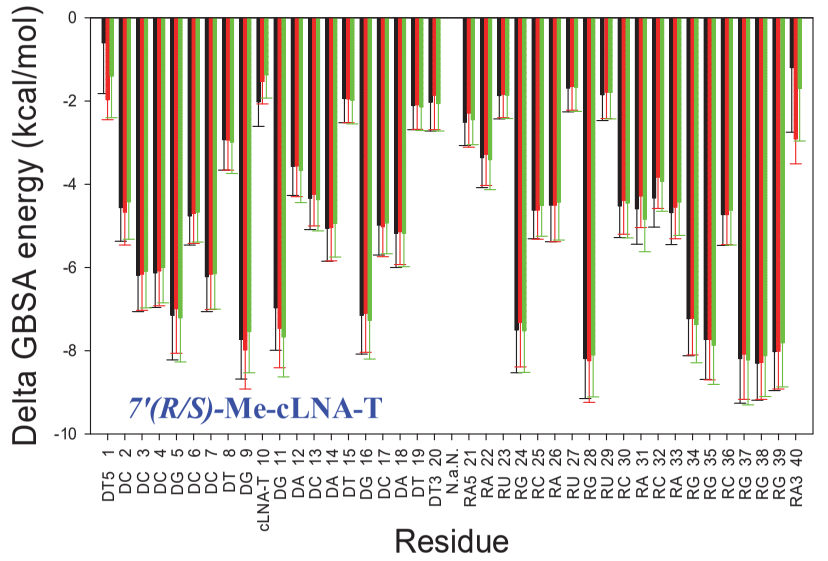

Delta GBSA energy (kcal/mol)
0
-2
-4
-6
-8
-10
7′(R/S)-Me-cLNA-T
DT5 1 DC 2 DC 3 DC 4 DG 5 DC 6 DC 7 DT 8 DG 9 cLNA-T 10 DG 11 DA 12 DC 13 DA 14 DT 15 DG 16 DC 17 DA 18 DT 19 DT3 20 N.a.N. RA5 21 RA 22 RU 23 RG 24 RC 25 RA 26 RU 27 RG 28 RU 29 RC 30 RA 31 RC 32 RA 33 RG 34 RG 35 RC 36 RG 37 RG 38 RG 39 RA3 40
Residue

Figure SIII.2. Pairwise comparison of the GBSA total energies (left column) and corresponding all heavy atoms root mean square deviations (RMSd, right column) along the MD trajectories of the *7'R*- and *7'S*-Me-cLNA modified duplexes in comparison with that of the native counterpart.

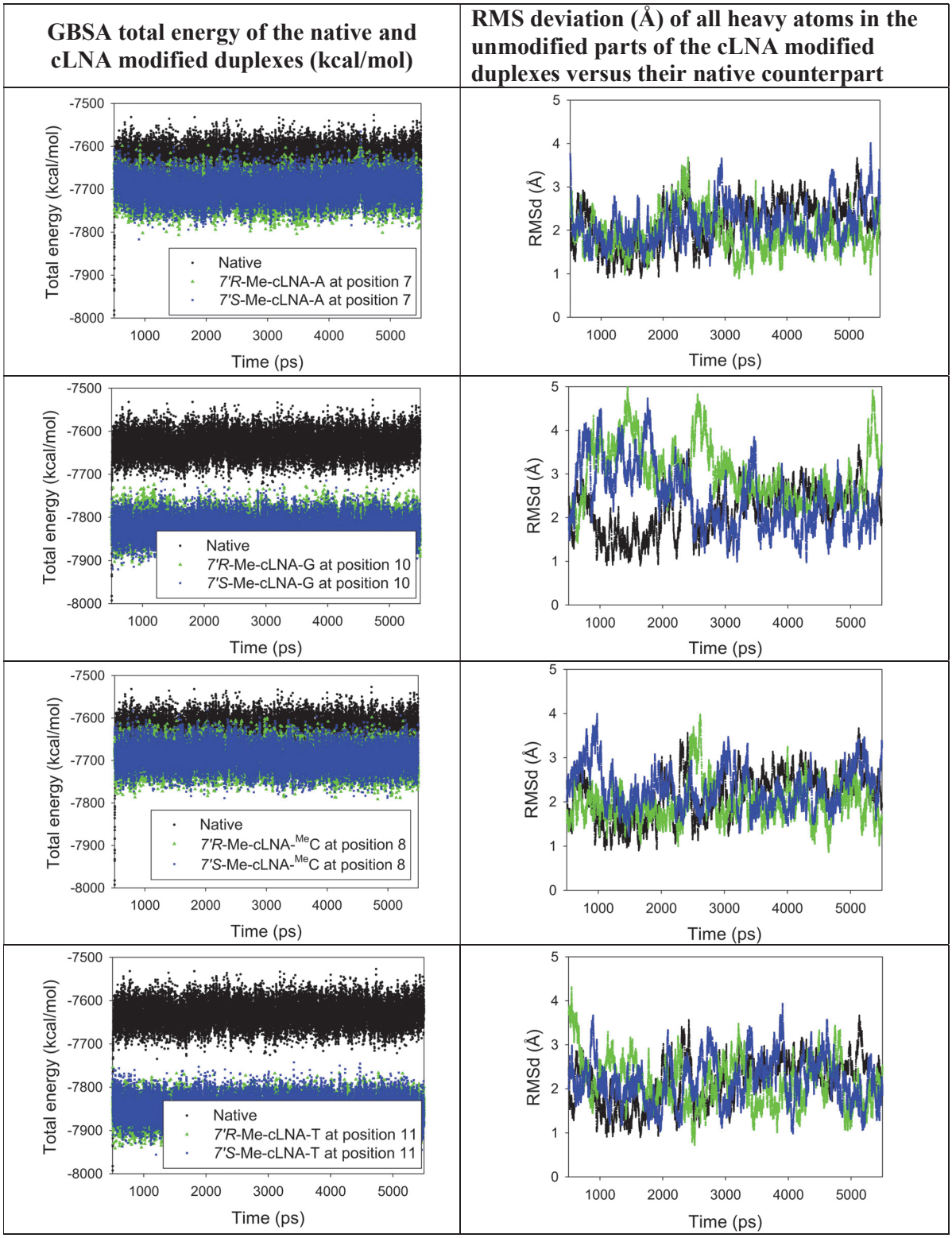


Table SIII.1. Total per-residue GBSA energy decomposition (kcal/mol) averaged along the 5 ns MD trajectory modeling the **native** AON-RNA duplex (AON1). Contributions from 1-4 interactions are added to the electrostatic and van der Waals energy components and Generalized Born approach is utilized to describe solvent contributions.

Residue	**Internal**		**van der Waals**		**Electrostatic**		**Polar Solv.**		**Non-Polar Solv.**		**TOTAL**	
	Avg.	***σ***	***Avg.***	***σ***	***Avg.***	***σ***	***Avg.***		***Avg.***	***σ***	***Avg.***	***σ***
DT5 1	43.50	4.09	1.62	2.51	20.68	7.56	-109.25	7.00	2.19	0.26	-41.26	3.96
DC 2	45.70	4.21	-4.01	2.12	29.01	12.10	-320.14	11.76	1.40	0.11	-248.03	4.17
DC 3	45.52	4.22	-6.44	1.71	49.81	10.86	-339.75	10.49	1.26	0.07	-249.60	4.03
DC 4	45.95	4.23	-6.41	1.73	64.96	10.25	-355.61	9.89	1.33	0.06	-249.77	4.05
DG 5	47.55	4.38	-12.22	1.62	117.97	11.10	-371.15	10.74	1.35	0.05	-216.51	4.21
DC 6	45.47	4.18	-6.37	1.70	84.19	9.41	-374.11	9.01	1.35	0.05	-249.47	3.95
DC 7	45.49	4.12	-7.16	1.67	93.12	9.00	-382.96	8.53	1.24	0.05	-250.28	3.89
DT 8	48.56	3.92	-8.79	1.61	226.88	7.99	-390.83	7.77	1.46	0.05	-122.72	4.02
DG 9	47.35	4.26	-12.77	1.64	146.07	9.10	-398.66	8.70	1.29	0.05	-216.73	4.14
DT 10	48.55	3.98	-8.96	1.63	230.35	7.70	-394.41	7.44	1.48	0.06	-122.99	4.16
DG 11	47.26	4.29	-11.88	1.69	143.88	8.50	-397.24	8.03	1.38	0.05	-216.59	4.20
DA 12	47.16	4.33	-11.01	1.59	180.63	7.31	-383.20	6.94	1.30	0.06	-165.12	4.16
DC 13	45.69	4.25	-5.86	1.75	85.15	6.87	-375.21	6.28	1.40	0.05	-248.83	4.02
DA 14	46.65	4.33	-11.50	1.54	164.54	5.48	-366.84	5.03	1.20	0.06	-165.95	4.23
DT 15	48.39	3.92	-8.41	1.65	198.38	5.11	-362.86	4.73	1.52	0.06	-122.98	4.07
DG 16	47.45	4.32	-11.99	1.63	101.36	5.54	-354.56	4.88	1.34	0.05	-216.41	4.23
DC 17	46.12	4.27	-6.49	1.74	46.16	5.41	-337.13	4.69	1.35	0.06	-250.00	3.97
DA 18	46.40	4.25	-11.42	1.55	119.82	5.08	-322.50	4.51	1.22	0.06	-166.49	4.12
DT 19	48.31	3.94	-9.12	1.62	144.03	4.63	-308.71	4.35	1.41	0.06	-124.08	4.05
DT3 20	47.09	3.92	-3.53	1.56	83.52	4.64	-218.05	4.39	2.29	0.06	-88.67	4.01
RA5 21	47.36	4.07	-2.80	1.56	-17.75	6.78	-105.48	6.20	1.88	0.05	-76.80	4.02
RA 22	50.47	4.24	-10.87	1.74	131.71	13.42	-341.35	12.76	1.31	0.06	-168.74	4.29
RU 23	46.53	3.79	-8.40	1.77	172.52	11.30	-363.41	10.83	1.34	0.05	-151.42	4.14
RG 24	51.50	4.35	-13.53	1.84	127.60	12.03	-387.45	11.11	1.33	0.06	-220.55	4.46
RC 25	49.35	4.19	-7.56	1.91	85.88	10.12	-382.26	9.48	1.32	0.05	-253.27	4.21
RA 26	50.72	4.24	-12.02	1.75	186.52	10.29	-394.79	9.66	1.29	0.05	-168.27	4.42
RU 27	46.59	3.81	-8.24	1.78	210.06	9.89	-400.83	9.52	1.36	0.05	-151.06	4.12
RG 28	51.92	4.39	-13.32	1.86	153.34	10.60	-413.39	9.77	1.33	0.05	-220.11	4.49
RU 29	46.95	3.77	-9.27	1.79	214.29	8.86	-404.03	8.49	1.27	0.05	-150.79	4.11
RC 30	49.24	4.18	-6.88	1.89	98.48	8.29	-394.66	7.61	1.35	0.05	-252.48	4.27
RA 31	50.53	4.21	-11.45	1.83	186.28	8.19	-394.68	7.46	1.31	0.06	-168.00	4.34
RC 32	49.05	4.15	-6.65	1.90	92.89	7.42	-389.48	6.71	1.37	0.04	-252.83	4.24
RA 33	49.91	4.23	-11.52	1.74	181.81	7.05	-390.43	6.40	1.34	0.05	-168.88	4.33
RG 34	51.08	4.28	-13.16	1.80	135.76	7.39	-396.36	6.56	1.38	0.05	-221.30	4.35
RG 35	51.38	4.30	-14.36	1.77	128.23	6.72	-388.33	5.81	1.29	0.05	-221.79	4.36
RC 36	48.87	4.11	-7.53	1.89	68.78	6.00	-365.21	5.11	1.33	0.05	-253.76	4.17
RG 37	51.07	4.30	-13.09	1.85	103.59	7.43	-364.45	6.57	1.39	0.06	-221.49	4.46
RG 38	51.10	4.31	-13.79	1.78	92.48	6.92	-353.70	5.99	1.37	0.05	-222.54	4.42
RG 39	51.06	4.22	-13.69	1.82	73.92	6.27	-335.61	5.37	1.33	0.05	-222.99	4.30
RA3 40	49.81	4.30	-5.29	1.68	52.15	6.73	-230.57	5.59	2.37	0.13	-131.53	4.48

Table SIII.2. Total delta per-residue GBSA energy decomposition (kcal/mol) averaged along the 5 ns MD trajectory modeling the **native** AON-RNA duplex (AON1). Contributions from 1-4 interactions are added to the electrostatic and van der Waals energy components and Generalized Born approach is utilized to describe solvent contributions.

Residue	**van der Waals**		**Electrostatic**		**Polar Solv.**		**Non-Polar Solv.**		**TOTAL**	
	Avg.	***σ***	***Avg.***	***σ***	***Avg.***	***σ***	***Avg.***	***σ***	***Avg.***	***σ***
DT5 1	-0.43	0.54	42.47	6.05	-42.52	5.39	-0.12	0.13	-0.60	1.22
DC 2	-1.86	0.88	120.71	8.82	-122.99	8.55	-0.41	0.09	-4.56	0.81
DC 3	-3.00	0.92	120.60	7.85	-123.41	7.62	-0.39	0.03	-6.19	0.87
DC 4	-2.97	0.92	126.73	6.86	-129.52	6.63	-0.38	0.03	-6.13	0.83
DG 5	-4.73	1.00	138.65	7.82	-140.51	7.60	-0.56	0.06	-7.15	1.07
DC 6	-1.42	0.88	143.67	6.63	-146.81	6.39	-0.21	0.03	-4.76	0.70
DC 7	-3.03	0.93	146.06	6.23	-148.86	6.01	-0.39	0.03	-6.22	0.84
DT 8	-3.53	0.79	159.24	5.68	-158.28	5.53	-0.36	0.04	-2.93	0.73
DG 9	-4.65	0.99	150.36	6.41	-152.87	6.21	-0.58	0.05	-7.73	0.95
DT 10	-1.75	0.69	162.15	6.24	-162.24	6.10	-0.18	0.04	-2.02	0.59
DG 11	-3.56	0.95	153.62	6.94	-156.56	6.60	-0.47	0.05	-6.97	1.02
DA 12	-3.04	0.75	155.22	6.42	-155.40	6.23	-0.36	0.05	-3.57	0.70
DC 13	-1.19	0.87	138.48	5.31	-141.41	4.93	-0.21	0.04	-4.34	0.75
DA 14	-4.80	0.87	137.27	3.90	-136.98	3.75	-0.54	0.05	-5.06	0.79
DT 15	-1.92	0.67	134.95	3.66	-134.76	3.40	-0.21	0.04	-1.94	0.58
DG 16	-4.25	0.96	119.90	3.86	-122.24	3.53	-0.55	0.05	-7.15	0.93
DC 17	-1.16	0.86	113.65	3.40	-117.29	3.02	-0.18	0.03	-4.98	0.72
DA 18	-4.58	0.82	111.26	2.94	-111.33	2.63	-0.53	0.05	-5.18	0.82
DT 19	-1.97	0.67	109.36	3.04	-109.26	2.75	-0.24	0.04	-2.11	0.58
DT3 20	-2.42	0.71	71.11	2.80	-70.31	2.47	-0.41	0.04	-2.03	0.69
RA5 21	-1.13	0.62	34.49	2.57	-35.57	2.35	-0.30	0.03	-2.51	0.56
RA 22	-2.79	0.73	135.38	8.21	-135.54	7.99	-0.41	0.04	-3.36	0.72
RU 23	-1.66	0.67	143.30	7.00	-143.31	6.81	-0.19	0.04	-1.87	0.56
RG 24	-4.39	1.01	140.86	7.46	-143.41	7.08	-0.56	0.05	-7.50	1.03
RC 25	-1.25	0.88	146.31	6.49	-149.50	6.26	-0.18	0.03	-4.62	0.69
RA 26	-4.49	0.83	154.70	6.66	-154.21	6.44	-0.50	0.04	-4.50	0.88
RU 27	-1.72	0.70	159.86	6.93	-159.63	6.72	-0.20	0.04	-1.69	0.57
RG 28	-4.50	1.02	150.40	7.58	-153.51	7.33	-0.58	0.05	-8.19	0.96
RU 29	-2.01	0.73	163.40	7.02	-163.03	6.82	-0.20	0.04	-1.85	0.62
RC 30	-2.01	0.92	149.64	6.07	-151.87	5.81	-0.28	0.04	-4.52	0.76
RA 31	-4.31	0.86	149.56	5.77	-149.36	5.56	-0.48	0.04	-4.59	0.85
RC 32	-1.19	0.88	139.16	5.24	-142.10	4.96	-0.21	0.04	-4.33	0.70
RA 33	-4.17	0.86	139.87	4.76	-139.90	4.50	-0.47	0.05	-4.68	0.77
RG 34	-3.09	0.95	125.44	4.51	-129.14	4.36	-0.43	0.04	-7.23	0.89
RG 35	-3.79	0.96	122.99	4.37	-126.47	4.07	-0.47	0.04	-7.73	0.96
RC 36	-1.38	0.87	123.92	3.26	-127.06	2.94	-0.21	0.03	-4.73	0.74
RG 37	-3.92	1.06	104.89	3.09	-108.68	2.91	-0.48	0.06	-8.19	1.07
RG 38	-3.02	0.94	98.44	3.31	-103.32	3.16	-0.39	0.04	-8.30	0.89
RG 39	-3.16	0.94	97.42	3.33	-101.86	3.09	-0.42	0.04	-8.02	0.94
RA3 40	-2.26	0.67	75.42	3.47	-74.08	2.76	-0.29	0.13	-1.20	1.55

Table SIII.3. Total per-residue GBSA energy decomposition (kcal/mol) averaged along the 5 ns MD trajectory modeling the ***7'R*-Me-cLNA-A modified at position 7** AON-RNA duplex (AON2). Contributions from 1-4 interactions are added to the electrostatic and van der Waals energy components and Generalized Born approach is utilized to describe solvent contributions.

Residue	**Internal**		**van der Waals**		**Electrostatic**		**Polar Solv.**		**Non-Polar Solv.**		**TOTAL**	
	Avg.	***σ***	***Avg.***	***σ***	***Avg.***	***σ***	***Avg.***	***σ***	***Avg.***	***σ***	***Avg.***	***σ***
DT5 1	45.03	3.82	-0.57	1.54	13.71	4.15	-102.73	3.91	1.91	0.06	-42.66	3.92
DC 2	45.33	4.19	-5.31	1.72	25.68	12.60	-316.44	12.26	1.34	0.05	-249.40	3.94
DC 3	45.48	4.13	-6.31	1.69	49.20	11.21	-339.64	10.82	1.30	0.05	-249.97	3.90
DC 4	45.76	4.15	-6.47	1.75	63.32	9.95	-353.91	9.64	1.33	0.06	-249.97	4.00
DG 5	47.52	4.27	-12.15	1.64	114.89	10.49	-368.13	10.09	1.35	0.05	-216.52	4.14
DC 6	45.76	4.25	-6.37	1.69	82.60	8.05	-372.52	7.60	1.35	0.05	-249.19	4.01
DC 7	45.56	4.15	-7.17	1.67	92.03	8.05	-381.94	7.56	1.24	0.05	-250.29	3.89
DT 8	48.34	3.97	-8.82	1.61	226.90	7.50	-390.87	7.29	1.46	0.05	-122.99	4.07
DG 9	47.43	4.26	-12.88	1.60	147.33	8.89	-399.93	8.52	1.28	0.05	-216.77	4.13
DT 10	48.24	3.90	-9.04	1.66	233.97	8.76	-398.00	8.42	1.47	0.07	-123.35	4.04
DG 11	47.16	4.27	-11.98	1.67	147.21	10.27	-400.47	9.81	1.38	0.05	-216.69	4.15
DA 12	47.13	4.24	-11.32	1.58	181.91	8.40	-384.03	7.93	1.29	0.06	-165.02	4.09
DC 13	46.25	4.25	-6.30	1.73	83.48	6.85	-373.31	6.13	1.42	0.05	-248.47	4.15
cLNA-A 14	**71.52**	**4.62**	**-7.65**	**2.08**	**66.60**	**5.67**	**-356.56**	**5.04**	**1.56**	**0.05**	**-224.53**	**4.64**
DT 15	50.13	4.00	-9.37	1.70	189.24	4.87	-366.46	4.51	1.32	0.05	-135.14	4.17
DG 16	47.62	4.27	-12.32	1.69	105.07	7.25	-358.18	6.58	1.31	0.05	-216.51	4.11
DC 17	45.83	4.21	-6.43	1.77	44.03	5.05	-334.86	4.31	1.34	0.06	-250.08	4.03
DA 18	46.62	4.35	-11.54	1.54	119.44	5.05	-322.01	4.47	1.21	0.06	-166.28	4.19
DT 19	47.77	3.88	-9.21	1.65	144.91	5.31	-309.63	4.99	1.37	0.07	-124.79	4.02
DT3 20	47.25	3.98	-3.75	1.61	84.31	5.07	-218.00	4.95	2.34	0.09	-87.85	4.13
RA5 21	47.91	4.13	-2.47	1.63	-16.65	7.82	-106.19	6.95	1.93	0.08	-75.48	4.20
RA 22	50.85	4.21	-10.97	1.80	136.21	15.95	-345.73	15.20	1.28	0.07	-168.36	4.30
RU 23	46.47	3.73	-8.40	1.78	175.02	14.56	-365.52	14.11	1.33	0.06	-151.09	4.02
RG 24	51.37	4.31	-13.23	1.85	129.34	16.23	-389.41	15.21	1.34	0.05	-220.58	4.41
RC 25	49.14	4.15	-7.39	1.88	86.09	12.36	-382.60	11.68	1.34	0.05	-253.42	4.18
RA 26	50.93	4.31	-11.45	1.78	185.32	11.31	-394.02	10.68	1.32	0.05	-167.91	4.40
RU 27	46.63	3.81	-8.46	1.73	209.55	9.43	-399.53	8.83	1.35	0.05	-150.46	4.13
RG 28	52.02	4.44	-13.68	1.86	150.14	10.90	-410.35	10.21	1.27	0.05	-220.61	4.59
RU 29	46.87	3.82	-9.53	1.75	211.65	8.08	-401.02	7.71	1.25	0.05	-150.78	4.14
RC 30	49.08	4.19	-6.93	1.90	96.72	7.94	-393.03	7.31	1.34	0.05	-252.82	4.29
RA 31	50.54	4.25	-11.50	1.85	185.39	8.70	-393.87	7.96	1.32	0.06	-168.12	4.42
RC 32	49.14	4.20	-6.66	1.90	92.76	7.99	-389.38	7.25	1.37	0.04	-252.77	4.26
RA 33	50.01	4.14	-11.43	1.80	180.85	7.41	-389.72	6.67	1.35	0.05	-168.93	4.28
RG 34	51.29	4.29	-13.12	1.80	133.68	7.72	-394.35	7.00	1.38	0.05	-221.12	4.40
RG 35	51.41	4.23	-14.37	1.78	127.07	7.39	-387.30	6.49	1.29	0.05	-221.90	4.34
RC 36	49.09	4.15	-7.48	1.89	68.36	5.82	-364.70	5.01	1.33	0.05	-253.40	4.20
RG 37	51.06	4.29	-13.03	1.85	102.05	7.36	-363.26	6.26	1.41	0.06	-221.78	4.46
RG 38	51.90	4.44	-13.61	1.79	89.28	8.23	-350.64	7.51	1.37	0.05	-221.71	4.59
RG 39	51.19	4.27	-13.70	1.77	71.47	6.55	-333.28	5.65	1.32	0.05	-223.00	4.35
RA3 40	50.08	4.30	-5.31	1.78	47.39	5.91	-227.27	5.15	2.24	0.06	-132.87	4.21

Table SIII.4. Total delta per-residue GBSA energy decomposition (kcal/mol) averaged along the 5 ns MD trajectory modeling the ***7′R*-Me-cLNA-A modified at position 7** AON-RNA duplex (AON2). Contributions from 1-4 interactions are added to the electrostatic and van der Waals energy components and Generalized Born approach is utilized to describe solvent contributions.

Residue	**van der Waals**		**Electrostatic**		**Polar Solv.**		**Non-Polar Solv.**		**TOTAL**	
	Avg.	***σ***	***Avg.***	***σ***	***Avg.***	***σ***	***Avg.***	***σ***	***Avg.***	***σ***
DT5 1	-0.79	0.64	35.69	2.73	-36.63	2.49	-0.26	0.02	-1.99	0.48
DC 2	-1.87	0.88	115.76	9.35	-118.26	9.10	-0.32	0.04	-4.70	0.80
DC 3	-2.99	0.93	119.81	8.14	-122.65	7.93	-0.39	0.04	-6.21	0.85
DC 4	-3.01	0.92	126.10	6.80	-128.81	6.58	-0.38	0.03	-6.10	0.84
DG 5	-4.74	1.00	137.42	7.52	-139.28	7.30	-0.56	0.05	-7.16	1.07
DC 6	-1.44	0.89	143.25	6.12	-146.35	5.90	-0.21	0.04	-4.75	0.70
DC 7	-3.06	0.92	145.71	5.92	-148.52	5.72	-0.40	0.03	-6.26	0.83
DT 8	-3.48	0.77	159.79	5.60	-158.86	5.47	-0.36	0.04	-2.91	0.71
DG 9	-4.64	0.97	151.76	6.42	-154.25	6.24	-0.58	0.05	-7.71	0.94
DT 10	-1.71	0.68	165.32	6.89	-165.41	6.68	-0.17	0.03	-1.97	0.61
DG 11	-3.45	0.94	156.50	8.08	-159.40	7.77	-0.46	0.05	-6.81	1.02
DA 12	-3.02	0.74	155.64	6.70	-155.62	6.48	-0.35	0.05	-3.34	0.68
DC 13	-1.22	0.87	137.53	5.01	-139.86	4.57	-0.21	0.04	-3.75	0.78
cLNA-A 14	**-5.47**	**0.78**	**136.26**	**3.49**	**-135.69**	**3.24**	**-0.56**	**0.05**	**-5.46**	**0.80**
DT 15	-2.04	0.74	137.44	3.25	-137.33	3.09	-0.24	0.04	-2.17	0.57
DG 16	-4.29	0.95	120.44	3.94	-122.90	3.59	-0.55	0.05	-7.30	0.91
DC 17	-1.13	0.89	112.61	3.23	-116.26	2.82	-0.19	0.03	-4.97	0.71
DA 18	-4.61	0.85	110.84	2.82	-110.73	2.49	-0.53	0.05	-5.04	0.83
DT 19	-1.91	0.66	110.84	3.18	-110.59	2.78	-0.24	0.04	-1.90	0.68
DT3 20	-2.11	0.79	72.56	2.88	-71.04	2.62	-0.35	0.09	-0.94	1.17
RA5 21	-0.86	0.56	36.92	3.38	-37.12	2.92	-0.25	0.07	-1.30	1.09
RA 22	-2.64	0.75	138.10	10.05	-138.01	9.76	-0.42	0.05	-2.97	0.90
RU 23	-1.65	0.68	144.37	9.56	-144.29	9.31	-0.20	0.04	-1.77	0.62
RG 24	-4.32	1.04	141.80	10.24	-144.48	9.80	-0.56	0.05	-7.55	1.04
RC 25	-1.27	0.87	146.41	7.87	-149.55	7.61	-0.18	0.03	-4.59	0.69
RA 26	-4.32	0.84	153.52	6.39	-153.29	6.24	-0.50	0.04	-4.59	0.82
RU 27	-2.22	0.65	158.98	5.55	-157.73	5.35	-0.23	0.04	-1.20	0.57
RG 28	-5.05	0.99	147.58	6.15	-151.02	5.95	-0.64	0.05	-9.14	0.98
RU 29	-2.20	0.72	161.17	5.79	-160.68	5.55	-0.21	0.04	-1.92	0.66
RC 30	-2.00	0.90	149.24	5.66	-151.35	5.35	-0.28	0.04	-4.39	0.77
RA 31	-4.24	0.87	149.97	5.80	-149.75	5.53	-0.48	0.04	-4.50	0.89
RC 32	-1.16	0.85	139.76	5.26	-142.73	4.98	-0.20	0.03	-4.32	0.69
RA 33	-4.05	0.86	139.54	4.52	-139.73	4.29	-0.46	0.04	-4.70	0.77
RG 34	-2.98	0.96	124.12	4.49	-127.91	4.36	-0.43	0.04	-7.20	0.89
RG 35	-3.79	0.97	122.05	4.41	-125.61	4.08	-0.47	0.04	-7.82	0.93
RC 36	-1.40	0.90	123.63	3.27	-126.72	2.94	-0.21	0.04	-4.70	0.72
RG 37	-3.96	1.06	104.84	3.03	-108.51	2.83	-0.48	0.06	-8.12	1.08
RG 38	-3.06	0.94	98.45	3.45	-103.28	3.29	-0.40	0.04	-8.29	0.88
RG 39	-3.32	0.94	98.19	3.38	-102.49	3.12	-0.42	0.04	-8.03	0.92
RA3 40	-2.50	0.75	72.64	2.83	-72.63	2.68	-0.42	0.04	-2.91	0.58

Table SIII.5. Total per-residue GBSA energy decomposition (kcal/mol) averaged along the 5 ns MD trajectory modeling the ***7′S*-Me-cLNA-A modified at position 7** AON-RNA duplex (AON5). Contributions from 1-4 interactions are added to the electrostatic and van der Waals energy components and Generalized Born approach is utilized to describe solvent contributions.

Residue	**Internal**		**van der Waals**		**Electrostatic**		**Polar Solv.**		**Non-Polar Solv.**		**TOTAL**	
	Avg.	***σ***	***Avg.***	***σ***	***Avg.***	***σ***	***Avg.***	***σ***	***Avg.***	***σ***	***Avg.***	***σ***
DT5 1	45.03	3.82	-0.57	1.54	13.71	4.15	-102.73	3.91	1.91	0.06	-42.66	3.92
DC 2	45.33	4.19	-5.31	1.72	25.68	12.60	-316.44	12.26	1.34	0.05	-249.40	3.94
DC 3	45.48	4.13	-6.31	1.69	49.20	11.21	-339.64	10.82	1.30	0.05	-249.97	3.90
DC 4	45.76	4.15	-6.47	1.75	63.32	9.95	-353.91	9.64	1.33	0.06	-249.97	4.00
DG 5	47.52	4.27	-12.15	1.64	114.89	10.49	-368.13	10.09	1.35	0.05	-216.52	4.14
DC 6	45.76	4.25	-6.37	1.69	82.60	8.05	-372.52	7.60	1.35	0.05	-249.19	4.01
DC 7	45.56	4.15	-7.17	1.67	92.03	8.05	-381.94	7.56	1.24	0.05	-250.29	3.89
DT 8	48.34	3.97	-8.82	1.61	226.90	7.50	-390.87	7.29	1.46	0.05	-122.99	4.07
DG 9	47.43	4.26	-12.88	1.60	147.33	8.89	-399.93	8.52	1.28	0.05	-216.77	4.13
DT 10	48.24	3.90	-9.04	1.66	233.97	8.76	-398.00	8.42	1.47	0.07	-123.35	4.04
DG 11	47.16	4.27	-11.98	1.67	147.21	10.27	-400.47	9.81	1.38	0.05	-216.69	4.15
DA 12	47.13	4.24	-11.32	1.58	181.91	8.40	-384.03	7.93	1.29	0.06	-165.02	4.09
DC 13	46.25	4.25	-6.30	1.73	83.48	6.85	-373.31	6.13	1.42	0.05	-248.47	4.15
cLNA-A 14	**71.52**	**4.62**	**-7.65**	**2.08**	**66.60**	**5.67**	**-356.56**	**5.04**	**1.56**	**0.05**	**-224.53**	**4.64**
DT 15	50.13	4.00	-9.37	1.70	189.24	4.87	-366.46	4.51	1.32	0.05	-135.14	4.17
DG 16	47.62	4.27	-12.32	1.69	105.07	7.25	-358.18	6.58	1.31	0.05	-216.51	4.11
DC 17	45.83	4.21	-6.43	1.77	44.03	5.05	-334.86	4.31	1.34	0.06	-250.08	4.03
DA 18	46.62	4.35	-11.54	1.54	119.44	5.05	-322.01	4.47	1.21	0.06	-166.28	4.19
DT 19	47.77	3.88	-9.21	1.65	144.91	5.31	-309.63	4.99	1.37	0.07	-124.79	4.02
DT3 20	47.25	3.98	-3.75	1.61	84.31	5.07	-218.00	4.95	2.34	0.09	-87.85	4.13
RA5 21	47.91	4.13	-2.47	1.63	-16.65	7.82	-106.19	6.95	1.93	0.08	-75.48	4.20
RA 22	50.85	4.21	-10.97	1.80	136.21	15.95	-345.73	15.20	1.28	0.07	-168.36	4.30
RU 23	46.47	3.73	-8.40	1.78	175.02	14.56	-365.52	14.11	1.33	0.06	-151.09	4.02
RG 24	51.37	4.31	-13.23	1.85	129.34	16.23	-389.41	15.21	1.34	0.05	-220.58	4.41
RC 25	49.14	4.15	-7.39	1.88	86.09	12.36	-382.60	11.68	1.34	0.05	-253.42	4.18
RA 26	50.93	4.31	-11.45	1.78	185.32	11.31	-394.02	10.68	1.32	0.05	-167.91	4.40
RU 27	46.63	3.81	-8.46	1.73	209.55	9.43	-399.53	8.83	1.35	0.05	-150.46	4.13
RG 28	52.02	4.44	-13.68	1.86	150.14	10.90	-410.35	10.21	1.27	0.05	-220.61	4.59
RU 29	46.87	3.82	-9.53	1.75	211.65	8.08	-401.02	7.71	1.25	0.05	-150.78	4.14
RC 30	49.08	4.19	-6.93	1.90	96.72	7.94	-393.03	7.31	1.34	0.05	-252.82	4.29
RA 31	50.54	4.25	-11.50	1.85	185.39	8.70	-393.87	7.96	1.32	0.06	-168.12	4.42
RC 32	49.14	4.20	-6.66	1.90	92.76	7.99	-389.38	7.25	1.37	0.04	-252.77	4.26
RA 33	50.01	4.14	-11.43	1.80	180.85	7.41	-389.72	6.67	1.35	0.05	-168.93	4.28
RG 34	51.29	4.29	-13.12	1.80	133.68	7.72	-394.35	7.00	1.38	0.05	-221.12	4.40
RG 35	51.41	4.23	-14.37	1.78	127.07	7.39	-387.30	6.49	1.29	0.05	-221.90	4.34
RC 36	49.09	4.15	-7.48	1.89	68.36	5.82	-364.70	5.01	1.33	0.05	-253.40	4.20
RG 37	51.06	4.29	-13.03	1.85	102.05	7.36	-363.26	6.26	1.41	0.06	-221.78	4.46
RG 38	51.90	4.44	-13.61	1.79	89.28	8.23	-350.64	7.51	1.37	0.05	-221.71	4.59
RG 39	51.19	4.27	-13.70	1.77	71.47	6.55	-333.28	5.65	1.32	0.05	-223.00	4.35
RA3 40	50.08	4.30	-5.31	1.78	47.39	5.91	-227.27	5.15	2.24	0.06	-132.87	4.21

Table SIII.6. Total delta per-residue GBSA energy decomposition (kcal/mol) averaged along the 5 ns MD trajectory modeling the ***7'S*-Me-cLNA-A modified at position 7** AON-RNA duplex (AON5). Contributions from 1-4 interactions are added to the electrostatic and van der Waals energy components and Generalized Born approach is utilized to describe solvent contributions.

Residue	**van der Waals**		**Electrostatic**		**Polar Solv.**		**Non-Polar Solv.**		**TOTAL**	
	Avg.	***σ***	***Avg.***	***σ***	***Avg.***	***σ***	***Avg.***	***σ***	***Avg.***	***σ***
DT5 1	-0.79	0.64	35.69	2.73	-36.63	2.49	-0.26	0.02	-1.99	0.48
DC 2	-1.87	0.88	115.76	9.35	-118.26	9.10	-0.32	0.04	-4.70	0.80
DC 3	-2.99	0.93	119.81	8.14	-122.65	7.93	-0.39	0.04	-6.21	0.85
DC 4	-3.01	0.92	126.10	6.80	-128.81	6.58	-0.38	0.03	-6.10	0.84
DG 5	-4.74	1.00	137.42	7.52	-139.28	7.30	-0.56	0.05	-7.16	1.07
DC 6	-1.44	0.89	143.25	6.12	-146.35	5.90	-0.21	0.04	-4.75	0.70
DC 7	-3.06	0.92	145.71	5.92	-148.52	5.72	-0.40	0.03	-6.26	0.83
DT 8	-3.48	0.77	159.79	5.60	-158.86	5.47	-0.36	0.04	-2.91	0.71
DG 9	-4.64	0.97	151.76	6.42	-154.25	6.24	-0.58	0.05	-7.71	0.94
DT 10	-1.71	0.68	165.32	6.89	-165.41	6.68	-0.17	0.03	-1.97	0.61
DG 11	-3.45	0.94	156.50	8.08	-159.40	7.77	-0.46	0.05	-6.81	1.02
DA 12	-3.02	0.74	155.64	6.70	-155.62	6.48	-0.35	0.05	-3.34	0.68
DC 13	-1.22	0.87	137.53	5.01	-139.86	4.57	-0.21	0.04	-3.75	0.78
cLNA-A 14	**-5.47**	**0.78**	**136.26**	**3.49**	**-135.69**	**3.24**	**-0.56**	**0.05**	**-5.46**	**0.80**
DT 15	-2.04	0.74	137.44	3.25	-137.33	3.09	-0.24	0.04	-2.17	0.57
DG 16	-4.29	0.95	120.44	3.94	-122.90	3.59	-0.55	0.05	-7.30	0.91
DC 17	-1.13	0.89	112.61	3.23	-116.26	2.82	-0.19	0.03	-4.97	0.71
DA 18	-4.61	0.85	110.84	2.82	-110.73	2.49	-0.53	0.05	-5.04	0.83
DT 19	-1.91	0.66	110.84	3.18	-110.59	2.78	-0.24	0.04	-1.90	0.68
DT3 20	-2.11	0.79	72.56	2.88	-71.04	2.62	-0.35	0.09	-0.94	1.17
RA5 21	-0.86	0.56	36.92	3.38	-37.12	2.92	-0.25	0.07	-1.30	1.09
RA 22	-2.64	0.75	138.10	10.05	-138.01	9.76	-0.42	0.05	-2.97	0.90
RU 23	-1.65	0.68	144.37	9.56	-144.29	9.31	-0.20	0.04	-1.77	0.62
RG 24	-4.32	1.04	141.80	10.24	-144.48	9.80	-0.56	0.05	-7.55	1.04
RC 25	-1.27	0.87	146.41	7.87	-149.55	7.61	-0.18	0.03	-4.59	0.69
RA 26	-4.32	0.84	153.52	6.39	-153.29	6.24	-0.50	0.04	-4.59	0.82
RU 27	-2.22	0.65	158.98	5.55	-157.73	5.35	-0.23	0.04	-1.20	0.57
RG 28	-5.05	0.99	147.58	6.15	-151.02	5.95	-0.64	0.05	-9.14	0.98
RU 29	-2.20	0.72	161.17	5.79	-160.68	5.55	-0.21	0.04	-1.92	0.66
RC 30	-2.00	0.90	149.24	5.66	-151.35	5.35	-0.28	0.04	-4.39	0.77
RA 31	-4.24	0.87	149.97	5.80	-149.75	5.53	-0.48	0.04	-4.50	0.89
RC 32	-1.16	0.85	139.76	5.26	-142.73	4.98	-0.20	0.03	-4.32	0.69
RA 33	-4.05	0.86	139.54	4.52	-139.73	4.29	-0.46	0.04	-4.70	0.77
RG 34	-2.98	0.96	124.12	4.49	-127.91	4.36	-0.43	0.04	-7.20	0.89
RG 35	-3.79	0.97	122.05	4.41	-125.61	4.08	-0.47	0.04	-7.82	0.93
RC 36	-1.40	0.90	123.63	3.27	-126.72	2.94	-0.21	0.04	-4.70	0.72
RG 37	-3.96	1.06	104.84	3.03	-108.51	2.83	-0.48	0.06	-8.12	1.08
RG 38	-3.06	0.94	98.45	3.45	-103.28	3.29	-0.40	0.04	-8.29	0.88
RG 39	-3.32	0.94	98.19	3.38	-102.49	3.12	-0.42	0.04	-8.03	0.92
RA3 40	-2.50	0.75	72.64	2.83	-72.63	2.68	-0.42	0.04	-2.91	0.58

Table SIII.7. Total per-residue GBSA energy decomposition (kcal/mol) averaged along the 5 ns MD trajectory modeling the ***7'R*-Me-cLNA-^{Me}C modified at position 8** AON-RNA duplex (AON14). Contributions from 1-4 interactions are added to the electrostatic and van der Waals energy components and Generalized Born approach is utilized to describe solvent contributions.

Residue	**Internal**		**van der Waals**		**Electrostatic**		**Polar Solv.**		**Non-Polar Solv.**		**TOTAL**	
	Avg.	***σ***	***Avg.***	***σ***	***Avg.***	***σ***	***Avg.***	***σ***	***Avg.***	***σ***	***Avg.***	***σ***
DT5 1	43.87	3.95	-0.48	1.68	14.28	4.71	-102.86	4.51	1.91	0.07	-43.28	3.88
DC 2	48.63	4.32	-5.13	1.74	17.11	10.00	-308.27	9.80	1.35	0.06	-246.31	4.12
DC 3	45.74	4.17	-6.23	1.70	48.81	10.25	-339.26	9.89	1.30	0.05	-249.65	3.96
DC 4	45.85	4.17	-6.46	1.74	66.38	8.95	-356.98	8.57	1.33	0.06	-249.87	4.01
DG 5	47.53	4.32	-12.13	1.65	119.32	10.03	-372.48	9.61	1.34	0.05	-216.42	4.19
DC 6	45.88	4.24	-6.36	1.71	87.06	9.34	-376.93	8.88	1.35	0.05	-249.02	4.00
DC 7	45.97	4.22	-7.15	1.69	94.15	8.18	-383.94	7.74	1.23	0.05	-249.74	3.98
DT 8	48.27	3.90	-8.87	1.61	227.31	7.51	-391.26	7.29	1.46	0.06	-123.09	4.03
DG 9	47.48	4.32	-12.74	1.63	145.53	8.77	-398.27	8.42	1.28	0.05	-216.71	4.20
DT 10	48.33	3.97	-8.89	1.64	227.69	7.22	-391.97	7.00	1.47	0.06	-123.36	4.08
DG 11	46.93	4.29	-12.14	1.64	140.65	8.02	-394.19	7.50	1.38	0.05	-217.38	4.18
DA 12	47.42	4.29	-11.53	1.53	179.72	7.20	-382.26	6.82	1.30	0.05	-165.35	4.13
cLNA-^{Me}C 13	**73.62**	**4.61**	**-2.09**	**2.41**	**4.01**	**7.11**	**-378.06**	**6.40**	**1.77**	**0.05**	**-300.75**	**4.66**
DA 14	47.28	4.28	-12.99	1.60	163.08	6.44	-376.72	6.09	1.06	0.06	-178.29	4.16
DT 15	48.19	3.97	-8.65	1.70	198.74	5.40	-363.20	5.05	1.46	0.08	-123.46	4.11
DG 16	47.42	4.24	-12.05	1.65	102.21	5.88	-355.42	5.22	1.34	0.05	-216.51	4.13
DC 17	45.97	4.21	-6.52	1.72	47.39	5.22	-338.14	4.48	1.35	0.06	-249.95	3.98
DA 18	46.41	4.23	-11.51	1.56	121.12	4.74	-323.73	4.15	1.22	0.06	-166.49	4.12
DT 19	47.76	3.91	-9.30	1.64	145.48	4.89	-310.21	4.58	1.37	0.07	-124.90	4.00
DT3 20	47.15	3.98	-3.72	1.57	84.68	4.78	-218.18	4.58	2.34	0.08	-87.74	4.22
RA5 21	47.94	4.15	-2.61	1.61	-16.23	7.13	-106.57	6.32	1.92	0.08	-75.55	4.13
RA 22	50.76	4.15	-11.11	1.73	135.92	13.76	-345.14	12.97	1.28	0.06	-168.29	4.27
RU 23	46.38	3.75	-8.39	1.78	173.24	11.55	-363.85	11.30	1.33	0.06	-151.30	4.08
RG 24	51.49	4.32	-13.42	1.84	127.55	12.53	-387.52	11.73	1.34	0.06	-220.56	4.44
RC 25	49.29	4.14	-7.41	1.90	86.40	9.82	-382.90	9.11	1.33	0.05	-253.29	4.17
RA 26	50.48	4.16	-11.84	1.77	187.56	9.67	-395.91	9.07	1.30	0.05	-168.41	4.32
RU 27	46.56	3.82	-8.37	1.75	211.99	9.24	-402.70	8.79	1.35	0.04	-151.17	4.19
RG 28	51.88	4.31	-13.73	1.79	157.64	10.03	-417.11	9.12	1.33	0.05	-219.99	4.41
RU 29	46.87	3.83	-9.50	1.72	216.05	8.17	-405.20	7.74	1.25	0.05	-150.51	4.11
RC 30	49.08	4.17	-6.93	1.86	99.00	7.76	-394.86	7.04	1.34	0.05	-252.38	4.22
RA 31	50.43	4.19	-11.59	1.82	184.98	7.57	-393.49	6.77	1.30	0.06	-168.37	4.36
RC 32	48.97	4.12	-6.76	1.86	89.46	6.72	-386.02	5.93	1.36	0.04	-252.98	4.18
RA 33	49.99	4.13	-11.52	1.77	177.46	6.34	-386.22	5.77	1.34	0.05	-168.95	4.26
RG 34	51.13	4.29	-13.08	1.79	131.55	6.82	-392.30	6.01	1.39	0.04	-221.31	4.35
RG 35	51.28	4.24	-14.42	1.77	125.68	6.63	-385.92	5.73	1.29	0.05	-222.10	4.30
RC 36	49.05	4.17	-7.55	1.88	68.81	5.50	-365.00	4.74	1.33	0.05	-253.36	4.14
RG 37	51.12	4.26	-13.08	1.88	103.42	6.34	-364.30	5.38	1.40	0.06	-221.44	4.37
RG 38	51.21	4.32	-13.72	1.77	92.41	6.28	-353.69	5.43	1.36	0.05	-222.43	4.41
RG 39	51.30	4.30	-13.64	1.83	72.71	6.32	-334.44	5.34	1.32	0.05	-222.76	4.41
RA3 40	49.86	4.25	-5.06	2.07	48.55	6.11	-228.23	5.23	2.24	0.09	-132.64	4.25

Table SIII.8. Total delta per-residue GBSA energy decomposition (kcal/mol) averaged along the 5 ns MD trajectory modeling the ***7'R*-Me-cLNA-^{Me}C modified at position 8** AON-RNA duplex (AON14). Contributions from 1-4 interactions are added to the electrostatic and van der Waals energy components and Generalized Born approach is utilized to describe solvent contributions.

Residue	**van der Waals**		**Electrostatic**		**Polar Solv.**		**Non-Polar Solv.**		**TOTAL**	
	Avg.	***σ***	***Avg.***	***σ***	***Avg.***	***σ***	***Avg.***	***σ***	***Avg.***	***σ***
DT5 1	-1.05	0.88	35.68	2.40	-36.27	2.37	-0.27	0.04	-1.91	0.56
DC 2	-1.72	0.92	108.95	7.62	-111.64	7.41	-0.30	0.05	-4.71	0.79
DC 3	-2.93	0.93	119.63	7.62	-122.45	7.43	-0.38	0.04	-6.13	0.88
DC 4	-2.95	0.92	127.92	6.27	-130.63	6.07	-0.38	0.03	-6.03	0.84
DG 5	-4.71	1.00	140.81	6.99	-142.63	6.81	-0.56	0.05	-7.09	1.04
DC 6	-1.45	0.88	146.42	6.69	-149.46	6.43	-0.21	0.03	-4.70	0.72
DC 7	-3.10	0.93	146.98	5.71	-149.76	5.49	-0.40	0.03	-6.28	0.84
DT 8	-3.52	0.76	159.73	5.43	-158.75	5.30	-0.36	0.03	-2.91	0.71
DG 9	-4.62	0.96	149.81	6.27	-152.38	6.01	-0.58	0.05	-7.77	0.92
DT 10	-1.65	0.69	160.62	5.88	-160.92	5.80	-0.17	0.03	-2.11	0.55
DG 11	-3.51	0.94	150.11	6.23	-153.57	5.92	-0.47	0.05	-7.44	1.00
DA 12	-3.15	0.71	153.35	5.69	-153.15	5.54	-0.36	0.04	-3.31	0.68
cLNA-^{Me}C 13	**-1.96**	**0.81**	**145.30**	**4.97**	**-146.98**	**4.65**	**-0.25**	**0.05**	**-3.88**	**0.78**
DA 14	-4.75	0.82	142.25	4.14	-141.90	3.96	-0.53	0.05	-4.94	0.78
DT 15	-1.88	0.69	135.02	3.65	-134.98	3.51	-0.22	0.04	-2.06	0.54
DG 16	-4.26	0.96	119.01	3.80	-121.45	3.44	-0.56	0.05	-7.26	0.93
DC 17	-1.18	0.86	113.73	3.38	-117.28	3.03	-0.19	0.03	-4.92	0.72
DA 18	-4.60	0.85	111.59	2.89	-111.53	2.59	-0.53	0.05	-5.07	0.83
DT 19	-1.94	0.65	110.95	3.25	-110.71	2.90	-0.24	0.04	-1.94	0.61
DT3 20	-2.06	0.72	72.46	2.81	-70.89	2.50	-0.35	0.08	-0.84	1.12
RA5 21	-0.87	0.61	36.72	2.78	-36.90	2.37	-0.25	0.07	-1.31	1.06
RA 22	-2.63	0.72	137.81	8.36	-137.77	8.20	-0.42	0.05	-3.00	0.75
RU 23	-1.62	0.69	143.85	8.02	-143.85	7.81	-0.20	0.04	-1.82	0.59
RG 24	-4.39	1.01	141.32	8.33	-143.98	7.96	-0.56	0.05	-7.61	1.03
RC 25	-1.26	0.88	147.14	6.33	-150.26	6.07	-0.18	0.03	-4.57	0.69
RA 26	-4.47	0.85	155.39	6.19	-155.03	5.97	-0.50	0.05	-4.61	0.84
RU 27	-1.78	0.70	161.06	5.91	-160.84	5.69	-0.20	0.04	-1.76	0.57
RG 28	-4.72	0.90	153.85	6.26	-156.33	6.06	-0.57	0.04	-7.78	0.96
RU 29	-2.24	0.67	164.24	5.97	-163.53	5.73	-0.21	0.04	-1.74	0.65
RC 30	-2.31	0.90	149.63	5.41	-151.17	5.04	-0.32	0.05	-4.16	0.79
RA 31	-4.41	0.85	147.95	4.90	-147.79	4.58	-0.49	0.04	-4.74	0.85
RC 32	-1.14	0.86	136.07	4.42	-139.14	4.09	-0.20	0.03	-4.41	0.67
RA 33	-4.11	0.84	136.10	4.12	-136.32	3.92	-0.46	0.04	-4.79	0.77
RG 34	-2.99	0.96	121.38	4.19	-125.22	4.04	-0.43	0.04	-7.25	0.86
RG 35	-3.85	0.96	120.22	4.19	-123.77	3.89	-0.48	0.04	-7.87	0.92
RC 36	-1.39	0.89	123.01	3.11	-126.14	2.80	-0.21	0.03	-4.72	0.70
RG 37	-3.95	1.06	103.91	3.04	-107.65	2.84	-0.49	0.06	-8.17	1.05
RG 38	-3.03	0.94	98.44	3.34	-103.25	3.20	-0.39	0.04	-8.23	0.89
RG 39	-3.38	0.96	98.55	3.37	-102.73	3.04	-0.42	0.05	-7.98	0.96
RA3 40	-2.48	0.99	73.69	2.88	-73.48	2.76	-0.42	0.08	-2.68	0.77

Table SIII.9. Total per-residue GBSA energy decomposition (kcal/mol) averaged along the 5 ns MD trajectory modeling the ***7′S*-Me-cLNA-^{Me}C modified at position 8** AON-RNA duplex (AON17). Contributions from 1-4 interactions are added to the electrostatic and van der Waals energy components and Generalized Born approach is utilized to describe solvent contributions.

Residue	**Internal**		**van der Waals**		**Electrostatic**		**Polar Solv.**		**Non-Polar Solv.**		**TOTAL**	
	Avg.	***σ***	***Avg.***	***σ***	***Avg.***	***σ***	***Avg.***	***σ***	***Avg.***	***σ***	***Avg.***	***σ***
DT5 1	41.96	3.77	0.32	2.37	8.14	6.02	-94.67	5.09	1.87	0.20	-42.38	3.89
DC 2	48.32	4.25	-3.29	1.85	8.07	8.28	-300.18	7.80	1.50	0.08	-245.58	4.06
DC 3	45.56	4.14	-6.34	1.70	47.19	10.08	-337.47	9.70	1.28	0.08	-249.78	3.95
DC 4	45.75	4.18	-6.60	1.77	63.42	8.88	-354.06	8.58	1.32	0.07	-250.18	4.01
DG 5	47.25	4.34	-12.16	1.66	113.88	9.35	-367.13	9.03	1.36	0.05	-216.80	4.17
DC 6	48.07	4.78	-6.14	1.71	83.28	8.58	-373.39	8.10	1.36	0.05	-246.83	4.61
DC 7	45.62	4.19	-7.01	1.69	94.89	9.60	-384.76	9.11	1.24	0.05	-250.03	3.98
DT 8	48.49	3.98	-8.81	1.60	227.96	8.42	-391.84	8.16	1.46	0.05	-122.74	4.07
DG 9	47.30	4.30	-12.82	1.62	146.49	9.26	-399.15	8.84	1.28	0.05	-216.90	4.17
DT 10	48.49	3.98	-8.87	1.63	228.50	7.53	-392.66	7.22	1.48	0.06	-123.07	4.10
DG 11	46.87	4.29	-12.14	1.63	141.18	8.64	-394.72	8.06	1.38	0.05	-217.42	4.16
DA 12	46.96	4.30	-11.48	1.51	178.83	7.37	-381.19	7.10	1.31	0.05	-165.56	4.13
cLNA-^{Me}C 13	**75.27**	**4.66**	**-2.05**	**2.37**	**-1.29**	**6.66**	**-374.67**	**5.92**	**1.78**	**0.05**	**-300.95**	**4.71**
DA 14	48.30	4.38	-13.07	1.58	161.20	6.58	-377.42	6.24	1.03	0.05	-179.97	4.24
DT 15	48.19	3.99	-8.74	1.66	199.87	6.02	-364.25	5.64	1.45	0.07	-123.48	4.12
DG 16	47.16	4.20	-12.09	1.66	101.31	6.32	-354.55	5.65	1.33	0.05	-216.84	4.12
DC 17	45.91	4.24	-6.47	1.73	46.73	5.56	-337.50	4.85	1.35	0.06	-249.98	4.04
DA 18	46.51	4.27	-11.48	1.53	121.09	5.66	-323.75	5.16	1.22	0.06	-166.41	4.11
DT 19	47.86	3.89	-9.18	1.67	145.58	5.34	-310.36	5.08	1.38	0.07	-124.71	4.03
DT3 20	47.38	3.93	-3.55	1.59	84.79	4.97	-218.69	4.64	2.33	0.08	-87.75	4.11
RA5 21	47.61	4.03	-2.63	1.58	-15.58	7.11	-107.34	6.32	1.91	0.07	-76.03	4.04
RA 22	50.62	4.22	-10.99	1.75	137.16	13.65	-346.59	12.82	1.30	0.07	-168.51	4.28
RU 23	46.57	3.91	-8.28	1.77	173.74	11.07	-364.67	10.45	1.34	0.06	-151.29	4.30
RG 24	52.04	4.54	-13.25	1.86	128.06	12.41	-388.15	11.76	1.34	0.05	-219.95	4.75
RC 25	49.2	4.1	-7.47	1.88	87.36	11.1	-	10.5	1.33	0.05	-	4.1

	9	8				6	383.88	2			253.37	5
RA 26	50.59	4.28	-12.06	1.73	187.98	10.83	-396.18	10.18	1.30	0.05	-168.38	4.37
RU 27	46.38	3.79	-8.31	1.75	210.97	9.75	-401.78	9.32	1.36	0.05	-151.38	4.08
RG 28	51.93	4.43	-13.53	1.80	154.86	10.34	-414.73	9.39	1.34	0.05	-220.14	4.53
RU 29	46.94	3.80	-9.49	1.69	212.78	7.48	-402.02	7.18	1.26	0.05	-150.53	4.10
RC 30	49.06	4.20	-6.94	1.88	95.35	7.07	-391.37	6.43	1.34	0.05	-252.57	4.24
RA 31	50.45	4.20	-11.60	1.82	182.08	7.28	-390.41	6.48	1.30	0.05	-168.18	4.35
RC 32	49.11	4.11	-6.74	1.89	87.59	7.07	-384.12	6.29	1.37	0.05	-252.79	4.18
RA 33	50.22	4.22	-11.49	1.75	176.03	6.91	-384.86	6.22	1.34	0.05	-168.76	4.28
RG 34	51.18	4.30	-13.02	1.82	130.49	7.34	-391.42	6.49	1.38	0.04	-221.38	4.41
RG 35	51.33	4.24	-14.47	1.78	125.33	6.62	-385.31	5.78	1.28	0.05	-221.85	4.34
RC 36	49.12	4.17	-7.41	1.92	69.30	5.80	-365.67	4.97	1.33	0.05	-253.33	4.26
RG 37	51.08	4.24	-12.99	1.89	103.69	6.76	-364.62	5.91	1.40	0.06	-221.44	4.38
RG 38	51.09	4.30	-13.82	1.76	92.40	6.80	-353.65	6.00	1.37	0.05	-222.61	4.42
RG 39	51.18	4.31	-13.47	1.95	72.72	6.53	-334.79	5.45	1.33	0.08	-223.03	4.40
RA3 40	51.06	4.57	-6.60	1.89	51.95	6.24	-228.05	5.62	2.07	0.17	-129.57	4.77

Table SIII.10. Total delta per-residue GBSA energy decomposition (kcal/mol) averaged along the 5 ns MD trajectory modeling the ***7'S*-Me-cLNA-** ^{Me}**C modified at position 8** AON-RNA duplex (AON17). Contributions from 1-4 interactions are added to the electrostatic and van der Waals energy components and Generalized Born approach is utilized to describe solvent contributions.

Residue	**van der Waals**		**Electrostatic**		**Polar Solv.**		**Non-Polar Solv.**		**TOTAL**	
	Avg.	***σ***	***Avg.***	***σ***	***Avg.***		***Avg.***	***σ***	***Avg.***	***σ***
DT5 1	-2.28	1.12	36.14	3.22	-34.75	2.76	-0.42	0.17	-1.31	1.15
DC 2	-1.76	0.95	103.23	5.75	-105.89	5.54	-0.40	0.08	-4.82	0.85
DC 3	-2.95	0.91	119.78	6.99	-122.60	6.78	-0.38	0.04	-6.15	0.85
DC 4	-2.95	0.93	126.55	6.07	-129.34	5.88	-0.38	0.03	-6.11	0.86
DG 5	-4.67	1.02	137.01	6.76	-138.79	6.61	-0.56	0.06	-7.00	1.09
DC 6	-1.44	0.86	142.95	6.19	-146.00	5.86	-0.21	0.04	-4.69	0.71
DC 7	-3.07	0.94	148.42	6.90	-151.14	6.65	-0.40	0.03	-6.19	0.86
DT 8	-3.54	0.76	161.08	6.19	-160.07	6.03	-0.36	0.03	-2.88	0.73
DG 9	-4.67	0.96	151.40	6.56	-153.90	6.35	-0.58	0.05	-7.76	0.94
DT 10	-1.72	0.68	161.89	5.92	-162.05	5.75	-0.17	0.03	-2.05	0.59
DG 11	-3.51	0.95	151.08	6.57	-154.55	6.24	-0.47	0.05	-7.44	1.00
DA 12	-3.13	0.71	153.46	5.75	-153.25	5.53	-0.36	0.04	-3.27	0.69
cLNA-^{Me}C 13	**-1.89**	**0.83**	**143.04**	**4.89**	**-144.66**	**4.57**	**-0.24**	**0.04**	**-3.75**	**0.80**
DA 14	-4.94	0.81	141.75	4.25	-141.23	3.99	-0.55	0.05	-4.97	0.78
DT 15	-1.88	0.68	135.98	3.98	-135.88	3.78	-0.21	0.04	-1.98	0.54
DG 16	-4.30	0.96	118.81	4.26	-121.28	3.92	-0.56	0.05	-7.32	0.91
DC 17	-1.21	0.88	113.65	3.49	-117.22	3.16	-0.19	0.03	-4.97	0.71
DA 18	-4.63	0.85	111.54	3.08	-111.52	2.78	-0.54	0.05	-5.14	0.83
DT 19	-1.91	0.65	110.61	3.41	-110.46	3.10	-0.24	0.04	-2.01	0.60
DT3 20	-2.10	0.76	72.39	2.97	-71.08	2.56	-0.36	0.08	-1.14	1.17
RA5 21	-0.92	0.59	36.68	3.21	-37.09	2.63	-0.26	0.06	-1.60	1.10
RA 22	-2.65	0.73	139.03	8.36	-139.02	8.04	-0.42	0.05	-3.05	0.78
RU 23	-1.59	0.68	144.67	7.04	-144.71	6.83	-0.19	0.04	-1.82	0.58
RG 24	-4.33	1.02	142.12	7.97	-144.81	7.69	-0.55	0.05	-7.58	1.00
RC 25	-1.30	0.88	147.58	7.39	-150.67	7.10	-0.18	0.03	-4.56	0.69
RA 26	-4.56	0.82	154.79	7.13	-154.47	6.90	-0.51	0.04	-4.75	0.84
RU 27	-1.79	0.68	160.05	6.84	-159.75	6.58	-0.20	0.03	-1.69	0.58
RG 28	-4.73	0.91	151.61	6.74	-154.40	6.50	-0.57	0.04	-8.09	0.94
RU 29	-2.25	0.67	160.92	5.87	-160.33	5.64	-0.21	0.04	-1.87	0.66
RC 30	-2.34	0.86	146.58	5.54	-148.09	5.16	-0.31	0.04	-4.16	0.82
RA 31	-4.44	0.83	145.48	5.40	-145.24	5.15	-0.50	0.04	-4.70	0.88
RC 32	-1.18	0.85	134.49	5.00	-137.50	4.68	-0.20	0.03	-4.39	0.68
RA 33	-4.13	0.86	135.00	4.47	-135.18	4.19	-0.46	0.04	-4.78	0.76
RG 34	-3.00	0.97	120.72	4.58	-124.62	4.41	-0.43	0.04	-7.34	0.87
RG 35	-3.99	0.97	120.20	4.21	-123.52	3.89	-0.49	0.04	-7.79	0.95
RC 36	-1.37	0.90	123.67	3.38	-126.80	3.03	-0.21	0.03	-4.71	0.72
RG 37	-3.83	1.12	104.03	3.20	-107.80	3.04	-0.48	0.06	-8.08	1.11
RG 38	-3.02	0.94	98.32	3.55	-103.17	3.39	-0.39	0.04	-8.26	0.92
RG 39	-3.22	1.00	97.95	3.33	-102.37	3.06	-0.43	0.07	-8.07	0.98
RA3 40	-3.90	1.43	76.88	3.16	-73.35	2.94	-0.59	0.19	-0.96	1.16

Table SIII.11. Total per-residue GBSA energy decomposition (kcal/mol averaged along the 5 ns MD trajectory modeling the ***7'R*-Me-cLNA-G modified at position 10** AON-RNA duplex (AON8). Contributions from 1-4 interactions are added to the electrostatic and van der Waals energy components and Generalized Born approach is utilized to describe solvent contributions.

Residue	**Internal**		**van der Waals**		**Electrostatic**		**Polar Solv.**		**Non-Polar Solv.**		**TOTAL**	
	Avg.	***σ***	***Avg.***	***σ***	***Avg.***	***σ***	***Avg.***	***σ***	***Avg.***	***σ***	***Avg.***	***σ***
DT5 1	45.00	3.98	-1.10	1.85	12.05	4.84	-99.91	4.76	1.89	0.12	-42.07	3.91
DC 2	46.00	4.25	-4.79	1.82	21.00	12.11	-311.75	11.93	1.36	0.06	-248.19	4.13
DC 3	45.82	4.16	-6.25	1.67	47.26	10.80	-337.79	10.43	1.32	0.06	-249.64	3.95
DC 4	45.64	4.20	-6.27	1.72	65.96	11.13	-356.56	10.82	1.35	0.06	-249.89	4.06
DG 5	47.67	4.31	-12.19	1.63	119.69	12.23	-373.08	11.84	1.34	0.05	-216.57	4.18
DC 6	45.59	4.23	-6.40	1.68	90.62	12.66	-380.35	12.23	1.35	0.05	-249.20	4.01
DC 7	45.55	4.16	-7.12	1.66	99.12	13.65	-388.92	13.20	1.25	0.05	-250.13	3.90
DT 8	48.50	4.03	-8.71	1.62	231.69	12.83	-395.61	12.48	1.47	0.05	-122.67	4.18
DG 9	47.61	4.27	-12.64	1.62	148.81	13.71	-401.87	13.19	1.30	0.05	-216.79	4.17
DT 10	48.85	3.96	-8.87	1.59	227.20	7.96	-392.16	7.72	1.53	0.06	-123.45	4.21
cLNA-G 11	**74.09**	**4.88**	**-7.38**	**2.20**	**-93.12**	**7.51**	**-381.91**	**6.65**	**1.69**	**0.05**	**-406.64**	**4.65**
DA 12	48.43	4.23	-11.91	1.60	179.43	6.75	-395.58	6.29	1.20	0.05	-178.43	4.17
DC 13	45.62	4.18	-6.08	1.77	90.07	6.53	-379.56	5.95	1.35	0.06	-248.60	3.95
DA 14	46.45	4.23	-11.91	1.65	166.76	6.62	-368.52	6.10	1.18	0.09	-166.03	4.13
DT 15	48.09	3.91	-9.88	1.83	201.39	5.33	-364.99	5.02	1.27	0.14	-124.12	4.12
DG 16	47.23	4.20	-14.42	2.19	107.25	6.06	-358.56	5.63	1.10	0.15	-217.39	4.20
DC 17	46.06	4.29	-7.71	1.96	50.16	7.57	-341.32	7.02	1.15	0.13	-251.66	4.19
DA 18	46.00	4.23	-11.80	1.63	123.72	6.89	-326.33	6.57	1.16	0.06	-167.24	4.13
DT 19	47.87	3.91	-9.41	1.69	148.96	5.99	-313.58	5.78	1.37	0.07	-124.79	4.05
DT3 20	47.21	3.98	-3.38	1.55	90.46	5.52	-223.44	5.36	2.53	0.08	-86.63	4.05
RA5 21	46.19	4.23	-3.52	3.19	-4.34	7.42	-115.89	5.72	1.32	0.42	-76.25	4.70
RA 22	54.12	4.30	-6.39	1.95	148.29	15.49	-359.03	14.34	1.49	0.09	-161.53	4.49
RU 23	47.25	3.87	-9.36	1.95	182.91	12.46	-372.31	11.85	1.19	0.07	-150.32	4.19
RG 24	51.51	4.29	-14.08	1.90	139.74	12.76	-398.29	11.87	1.31	0.06	-219.81	4.47
RC 25	49.6	4.2	-7.59	1.90	94.00	13.2	-	12.7	1.33	0.05	-	4.2

	0	3				8	390.42	4			253.09	8
RA 26	50.45	4.21	-12.28	1.71	198.14	15.36	-405.92	14.72	1.29	0.05	-168.31	4.36
RU 27	46.35	3.76	-8.35	1.76	220.81	14.51	-411.19	13.96	1.35	0.04	-151.04	4.13
RG 28	51.46	4.33	-13.27	1.86	161.09	13.69	-421.04	12.83	1.34	0.05	-220.43	4.49
RU 29	46.50	3.73	-8.76	1.74	215.84	9.63	-405.73	9.20	1.29	0.05	-150.85	4.04
RC 30	49.09	4.15	-7.20	1.82	100.60	8.64	-394.09	7.85	1.35	0.05	-250.24	4.21
RA 31	50.50	4.18	-11.98	1.75	185.34	8.28	-393.04	7.48	1.26	0.05	-167.92	4.29
RC 32	49.23	4.14	-6.81	1.88	91.03	6.78	-386.87	6.09	1.35	0.05	-252.06	4.21
RA 33	49.95	4.18	-11.34	1.77	178.26	6.89	-387.19	6.20	1.36	0.05	-168.96	4.32
RG 34	51.33	4.37	-13.07	1.80	131.12	7.41	-392.02	6.72	1.39	0.04	-221.25	4.48
RG 35	51.31	4.25	-14.20	1.78	124.83	7.44	-385.32	6.52	1.30	0.05	-222.08	4.33
RC 36	49.09	4.14	-7.24	1.92	69.92	7.32	-366.15	6.63	1.35	0.06	-253.04	4.22
RG 37	51.34	4.34	-13.09	1.85	105.70	7.77	-366.46	7.02	1.39	0.06	-221.11	4.45
RG 38	50.91	4.22	-13.75	1.77	93.96	7.65	-355.19	6.78	1.37	0.05	-222.70	4.28
RG 39	51.53	4.47	-13.13	2.01	72.42	8.07	-334.60	7.02	1.36	0.08	-222.42	4.57
RA3 40	50.01	4.33	-6.89	2.38	51.03	6.43	-228.02	5.83	2.08	0.20	-131.78	4.48

Table SIII.12. Total delta per-residue GBSA energy decomposition (kcal/mol) averaged along the 5 ns MD trajectory modeling the ***7′R*-Me-cLNA-G modified at position 10** AON-RNA duplex (AON8). Contributions from 1-4 interactions are added to the electrostatic and van der Waals energy components and Generalized Born approach is utilized to describe solvent contributions.

Residue	**van der Waals**		**Electrostatic**		**Polar Solv.**		**Non-Polar Solv.**		**TOTAL**	
	Avg.	σ	***Avg.***	σ	***Avg.***	σ	***Avg.***	□	***Avg.***	σ
DT5 1	-2.40	1.63	36.49	3.64	-35.57	3.70	-0.37	0.15	-1.84	1.25
DC 2	-1.86	0.94	113.94	8.15	-116.51	7.96	-0.38	0.06	-4.81	0.92
DC 3	-2.83	0.93	118.62	7.75	-121.46	7.57	-0.37	0.04	-6.04	0.85
DC 4	-2.87	0.93	128.10	7.89	-130.82	7.65	-0.37	0.03	-5.96	0.86
DG 5	-4.93	1.06	140.36	8.81	-142.33	8.64	-0.58	0.06	-7.48	1.13
DC 6	-1.58	0.90	148.20	9.21	-151.06	8.95	-0.22	0.04	-4.66	0.74
DC 7	-3.13	0.91	150.16	9.69	-152.85	9.43	-0.40	0.03	-6.22	0.84
DT 8	-3.44	0.78	162.93	9.05	-161.93	8.83	-0.35	0.04	-2.79	0.72
DG 9	-4.40	1.00	152.83	9.41	-155.80	9.11	-0.56	0.05	-7.93	1.00
DT 10	-1.98	0.77	162.31	6.03	-162.14	5.83	-0.19	0.04	-2.00	0.60
cLNA-G 11	**-4.87**	**0.87**	**153.44**	**5.05**	**-155.12**	**4.77**	**-0.51**	**0.04**	**-7.06**	**0.83**
DA 12	-3.53	0.74	162.05	5.43	-161.69	5.21	-0.40	0.04	-3.57	0.78
DC 13	-1.23	0.90	142.14	5.11	-144.89	4.71	-0.21	0.05	-4.18	0.75
DA 14	-5.14	1.03	139.66	4.96	-138.81	4.73	-0.57	0.08	-4.86	0.83
DT 15	-3.51	1.05	137.31	3.92	-136.33	3.76	-0.46	0.14	-2.99	0.87
DG 16	-6.81	1.81	124.32	3.78	-124.68	3.48	-0.80	0.15	-7.97	1.45
DC 17	-2.42	1.22	115.84	4.31	-119.72	3.91	-0.38	0.12	-6.67	1.45
DA 18	-4.54	0.90	114.05	3.77	-114.47	3.64	-0.54	0.06	-5.51	1.05
DT 19	-1.62	0.68	113.61	3.69	-113.64	3.38	-0.22	0.04	-1.86	0.60
DT3 20	-1.62	0.60	76.92	2.97	-74.87	2.97	-0.16	0.06	0.27	0.42
RA5 21	-6.21	2.54	47.16	3.47	-43.85	2.87	-0.93	0.31	-3.82	2.46
RA 22	-2.88	0.78	151.82	8.68	-150.82	8.32	-0.53	0.07	-2.41	0.93
RU 23	-1.62	0.71	149.67	7.40	-149.76	7.13	-0.19	0.04	-1.89	0.63
RG 24	-4.23	1.02	145.95	7.47	-148.30	7.22	-0.52	0.05	-7.10	1.12
RC 25	-1.07	0.84	151.17	9.01	-154.50	8.74	-0.16	0.03	-4.56	0.81
RA 26	-4.55	0.82	160.83	10.81	-160.27	10.42	-0.51	0.04	-4.50	0.93
RU 27	-1.73	0.69	164.81	10.05	-164.53	9.71	-0.20	0.03	-1.64	0.60
RG 28	-4.34	1.02	152.43	9.26	-155.70	8.88	-0.57	0.05	-8.18	1.02
RU 29	-1.72	0.72	161.40	6.92	-161.43	6.73	-0.18	0.04	-1.93	0.67
RC 30	-2.83	0.74	149.61	6.03	-148.70	5.76	-0.32	0.03	-2.24	0.77
RA 31	-5.08	0.83	144.82	5.44	-144.32	5.20	-0.55	0.04	-5.12	0.74
RC 32	-1.53	0.93	134.44	4.71	-136.91	4.42	-0.24	0.05	-4.24	0.75
RA 33	-4.20	0.89	135.65	4.31	-135.78	4.08	-0.46	0.05	-4.79	0.81
RG 34	-3.00	0.94	121.57	4.45	-125.34	4.34	-0.42	0.04	-7.19	0.87
RG 35	-3.68	0.96	119.93	4.49	-123.73	4.17	-0.47	0.04	-7.95	0.93
RC 36	-1.49	0.91	123.48	3.68	-126.38	3.41	-0.22	0.04	-4.61	0.77
RG 37	-4.33	1.14	105.35	3.41	-108.91	3.23	-0.52	0.07	-8.41	1.15
RG 38	-3.07	0.93	99.67	3.46	-104.36	3.32	-0.39	0.04	-8.15	0.93
RG 39	-2.99	1.00	97.77	3.81	-102.34	3.42	-0.39	0.06	-7.95	0.99
RA3 40	-4.17	1.95	75.74	3.07	-72.73	3.00	-0.60	0.22	-1.75	1.35

Table SIII.13. Total per-residue GBSA energy decomposition (kcal/mol) averaged along the 5 ns MD trajectory modeling the ***7′S*-Me-cLNA-G modified at position 10** AON-RNA duplex (AON11). Contributions from 1-4 interactions are added to the electrostatic and van der Waals energy components and Generalized Born approach is utilized to describe solvent contributions.

Residue	**Internal**		**van der Waals**		**Electrostatic**		**Polar Solv.**		**Non-Polar Solv.**		**TOTAL**	
	Avg.	**σ**	***Avg.***	**σ**	***Avg.***	**σ**	***Avg.***	**σ**	***Avg.***	**σ**	***Avg.***	**σ**
DT5 1	44.96	3.79	-0.63	1.56	14.45	4.10	-103.38	3.89	1.90	0.07	-42.71	3.90
DC 2	45.53	4.18	-5.31	1.73	27.31	14.45	-318.04	14.03	1.35	0.06	-249.16	4.00
DC 3	45.65	4.19	-6.27	1.67	51.96	13.26	-342.36	12.88	1.30	0.05	-249.72	3.97
DC 4	45.95	4.25	-6.29	1.72	68.45	12.44	-359.02	12.11	1.34	0.06	-249.57	4.06
DG 5	47.50	4.35	-12.23	1.64	123.30	14.49	-376.44	14.08	1.35	0.05	-216.53	4.20
DC 6	45.50	4.17	-6.41	1.70	93.45	14.48	-383.16	14.04	1.35	0.05	-249.27	3.98
DC 7	45.55	4.16	-7.19	1.65	103.09	14.55	-392.74	14.05	1.24	0.05	-250.05	3.89
DT 8	48.52	3.92	-8.85	1.63	235.39	12.85	-399.26	12.52	1.46	0.06	-122.74	4.01
DG 9	47.21	4.37	-12.52	1.64	152.51	12.15	-405.44	11.73	1.31	0.05	-216.94	4.25
DT 10	48.88	4.10	-8.08	1.64	231.26	9.67	-396.13	9.49	1.56	0.07	-122.51	4.08
cLNA-G 11	**74.32**	**4.95**	**-7.21**	**2.32**	**-69.39**	**10.49**	**-402.52**	**9.50**	**1.71**	**0.06**	**-403.08**	**4.76**
DA 12	48.65	4.22	-12.13	1.60	181.90	7.98	-397.40	7.67	1.14	0.05	-177.84	4.17
DC 13	45.67	4.24	-6.00	1.74	89.39	7.86	-379.05	7.39	1.37	0.05	-248.63	3.98
DA 14	46.43	4.22	-11.47	1.53	164.74	6.39	-367.10	6.06	1.21	0.06	-166.18	4.09
DT 15	48.38	3.98	-8.44	1.65	199.99	5.86	-364.47	5.53	1.52	0.06	-123.02	4.05
DG 16	47.28	4.25	-12.08	1.64	104.10	6.61	-357.27	6.04	1.34	0.05	-216.64	4.13
DC 17	46.08	4.31	-6.60	1.71	51.23	7.01	-341.96	6.50	1.35	0.06	-249.91	4.04
DA 18	46.71	4.28	-11.48	1.56	125.05	6.35	-327.71	5.91	1.21	0.06	-166.23	4.14
DT 19	47.95	3.95	-9.01	1.69	148.44	5.77	-313.26	5.45	1.42	0.07	-124.45	4.06
DT3 20	49.35	4.36	-3.46	1.61	85.02	6.02	-219.93	5.73	2.27	0.07	-86.75	4.33
RA5 21	47.49	4.13	-2.63	1.56	-17.67	6.60	-105.51	5.86	1.90	0.06	-76.43	4.03
RA 22	50.32	4.20	-10.73	1.78	129.50	12.44	-339.18	11.76	1.31	0.06	-168.77	4.31
RU 23	46.37	3.80	-8.11	1.79	171.22	10.90	-362.34	10.37	1.36	0.05	-151.50	4.10
RG 24	51.38	4.27	-13.35	1.84	130.01	12.42	-389.97	11.58	1.34	0.05	-220.59	4.43
RC 25	49.25	4.13	-7.49	1.89	93.66	12.49	-389.99	11.89	1.32	0.05	-253.25	4.18
RA 26	50.62	4.26	-12.09	1.74	197.75	14.37	-405.52	13.74	1.29	0.05	-167.95	4.39
RU 27	46.43	3.77	-8.24	1.74	222.29	15.15	-412.71	14.57	1.35	0.05	-150.88	4.11
RG 28	51.30	4.30	-13.28	1.88	165.49	16.13	-425.43	15.19	1.34	0.06	-220.58	4.42
RU 29	46.49	3.76	-8.80	1.73	220.53	12.81	-410.24	12.26	1.30	0.04	-150.73	4.06
RC 30	49.16	4.15	-7.25	1.86	103.63	9.77	-397.22	9.19	1.34	0.05	-250.34	4.24
RA 31	50.73	4.27	-12.32	1.73	187.77	8.69	-395.10	8.07	1.23	0.05	-167.70	4.35
RC 32	49.08	4.13	-6.90	1.88	91.68	7.56	-387.45	6.84	1.34	0.05	-252.24	4.17
RA 33	49.98	4.18	-11.44	1.77	178.52	7.98	-387.31	7.49	1.35	0.05	-168.90	4.29
RG 34	51.12	4.28	-13.03	1.79	132.38	8.52	-393.22	7.81	1.39	0.05	-221.36	4.36
RG 35	51.35	4.28	-14.25	1.80	127.21	8.69	-387.48	7.81	1.29	0.05	-221.88	4.41
RC 36	49.20	4.11	-7.50	1.92	71.84	7.11	-368.05	6.60	1.33	0.06	-253.19	4.17
RG 37	50.99	4.28	-13.15	1.86	107.02	7.47	-367.74	6.61	1.39	0.06	-221.49	4.44
RG 38	51.09	4.22	-13.77	1.78	95.11	7.64	-356.38	6.83	1.36	0.05	-222.58	4.31
RG 39	51.28	4.27	-13.60	1.84	74.76	7.55	-336.51	6.76	1.33	0.05	-222.74	4.37
RA3 40	50.16	4.31	-5.07	1.92	48.45	7.00	-228.48	6.25	2.25	0.07	-132.69	4.25

Table SIII.14. Total delta per-residue GBSA energy decomposition (kcal/mol) averaged along the 5 ns MD trajectory modeling the ***7′S*-Me-cLNA-G modified at position 10** AON-RNA duplex (AON11). Contributions from 1-4 interactions are added to the electrostatic and van der Waals energy components and Generalized Born approach is utilized to describe solvent contributions.

Residue	**van der Waals**		**Electrostatic**		**Polar Solv.**		**Non-Polar Solv.**		**TOTAL**	
	Avg.	***σ***	***Avg.***	***σ***	***Avg.***	***σ***	***Avg.***	***σ***	***Avg.***	***σ***
DT5 1	-0.83	0.65	36.59	2.70	-37.44	2.47	-0.26	0.03	-1.94	0.54
DC 2	-1.81	0.90	117.43	10.89	-119.96	10.54	-0.31	0.04	-4.66	0.82
DC 3	-2.94	0.94	121.57	9.71	-124.37	9.48	-0.38	0.04	-6.13	0.87
DC 4	-2.93	0.92	129.14	8.59	-131.86	8.37	-0.38	0.03	-6.03	0.83
DG 5	-4.76	1.03	142.65	10.07	-144.49	9.79	-0.56	0.06	-7.16	1.11
DC 6	-1.51	0.90	150.14	10.34	-153.06	10.06	-0.22	0.04	-4.64	0.76
DC 7	-3.14	0.93	152.55	10.23	-155.19	9.92	-0.40	0.03	-6.18	0.87
DT 8	-3.48	0.77	164.74	8.99	-163.70	8.75	-0.35	0.03	-2.79	0.72
DG 9	-4.31	0.99	154.15	8.09	-156.97	7.79	-0.55	0.05	-7.69	1.02
DT 10	-1.77	0.70	163.24	6.78	-163.14	6.62	-0.18	0.04	-1.86	0.58
cLNA-G 11	**-4.80**	**0.91**	**159.41**	**7.22**	**-160.83**	**6.95**	**-0.51**	**0.05**	**-6.73**	**0.90**
DA 12	-3.45	0.74	157.80	6.13	-157.51	5.98	-0.39	0.04	-3.56	0.80
DC 13	-1.16	0.88	139.46	5.75	-142.41	5.46	-0.20	0.05	-4.31	0.75
DA 14	-4.64	0.87	135.85	4.02	-135.61	3.93	-0.54	0.05	-4.94	0.79
DT 15	-1.89	0.68	134.01	3.53	-133.87	3.33	-0.21	0.04	-1.96	0.58
DG 16	-4.25	0.96	119.79	3.75	-122.22	3.43	-0.55	0.05	-7.23	0.92
DC 17	-1.21	0.86	115.03	3.70	-118.57	3.35	-0.19	0.03	-4.94	0.72
DA 18	-4.73	0.86	112.96	3.22	-112.81	2.95	-0.54	0.05	-5.12	0.85
DT 19	-1.90	0.66	111.07	3.27	-111.05	2.94	-0.22	0.05	-2.10	0.60
DT3 20	-2.30	0.70	71.46	3.27	-70.56	2.96	-0.41	0.05	-1.80	0.80
RA5 21	-1.14	0.61	34.75	3.01	-35.62	2.49	-0.29	0.04	-2.31	0.83
RA 22	-2.84	0.73	134.86	7.72	-134.94	7.42	-0.42	0.05	-3.34	0.85
RU 23	-1.49	0.67	143.93	6.90	-144.11	6.68	-0.18	0.04	-1.85	0.56
RG 24	-4.35	1.01	144.27	8.33	-146.92	7.99	-0.56	0.05	-7.56	1.04
RC 25	-1.29	0.87	152.95	8.69	-155.97	8.42	-0.18	0.03	-4.49	0.69
RA 26	-4.55	0.83	163.02	10.22	-162.29	9.89	-0.51	0.04	-4.33	0.92
RU 27	-1.75	0.71	168.92	10.71	-168.51	10.39	-0.20	0.04	-1.54	0.61
RG 28	-4.43	1.02	158.75	11.47	-161.79	11.08	-0.58	0.05	-8.04	1.05
RU 29	-1.79	0.73	167.57	9.36	-167.39	9.05	-0.18	0.04	-1.79	0.72
RC 30	-2.82	0.73	153.87	6.86	-152.84	6.60	-0.33	0.03	-2.13	0.78
RA 31	-5.13	0.85	148.32	5.67	-147.69	5.48	-0.56	0.05	-5.06	0.87
RC 32	-1.38	0.90	135.93	5.30	-138.55	4.98	-0.22	0.04	-4.22	0.74
RA 33	-3.94	0.86	136.36	5.44	-136.58	5.16	-0.44	0.05	-4.60	0.80
RG 34	-2.94	0.95	122.03	5.35	-125.82	5.20	-0.42	0.04	-7.14	0.87
RG 35	-3.76	0.96	121.10	5.10	-124.70	4.73	-0.47	0.04	-7.84	0.96
RC 36	-1.48	0.90	124.40	3.76	-127.38	3.56	-0.22	0.04	-4.68	0.79
RG 37	-4.03	1.09	105.50	3.28	-109.20	3.12	-0.49	0.06	-8.22	1.10
RG 38	-3.02	0.94	99.72	3.44	-104.52	3.27	-0.39	0.04	-8.21	0.90
RG 39	-3.28	0.94	99.29	3.44	-103.53	3.22	-0.41	0.04	-7.94	0.96
RA3 40	-2.41	0.78	73.50	2.86	-73.52	2.67	-0.41	0.05	-2.85	0.67

Table SIII.15. Total per-residue GBSA energy decomposition (kcal/mol) averaged along the 5 ns MD trajectory modeling the ***7′R*-Me-cLNA-T modified at position 11** AON-RNA duplex (AON20). Contributions from 1-4 interactions are added to the electrostatic and van der Waals energy components and Generalized Born approach is utilized to describe solvent contributions.

Residue	**Internal**		**van der Waals**		**Electrostatic**		**Polar Solv.**		**Non-Polar Solv.**		**TOTAL**	
	Avg.	***σ***	***Avg.***	***σ***	***Avg.***	***σ***	***Avg.***	***σ***	***Avg.***	***σ***	***Avg.***	***σ***
DT5 1	45.16	3.83	-0.49	1.52	14.87	3.92	-103.94	3.76	1.91	0.06	-42.49	3.92
DC 2	45.38	4.17	-5.32	1.71	30.52	11.79	-321.23	11.44	1.34	0.05	-249.30	3.94
DC 3	45.61	4.19	-6.31	1.69	54.29	10.55	-344.66	10.16	1.29	0.05	-249.77	3.95
DC 4	45.83	4.13	-6.51	1.72	69.62	8.91	-360.23	8.55	1.33	0.06	-249.96	3.94
DG 5	47.43	4.26	-12.18	1.65	123.00	9.71	-375.99	9.33	1.35	0.05	-216.39	4.16
DC 6	45.91	4.27	-6.43	1.72	90.04	9.39	-379.87	8.86	1.34	0.05	-249.00	4.02
DC 7	45.61	4.16	-7.19	1.68	97.20	9.13	-386.92	8.61	1.24	0.05	-250.07	3.96
DT 8	48.42	3.96	-9.06	1.61	229.00	7.89	-393.01	7.61	1.45	0.06	-123.20	4.06
DG 9	47.49	4.26	-12.67	1.63	144.74	9.53	-398.59	9.16	1.30	0.05	-217.73	4.12
cLNA-T 10	**74.18**	**4.67**	**-3.59**	**2.28**	**-10.70**	**9.13**	**-399.48**	**8.48**	**1.77**	**0.04**	**-337.82**	**4.50**
DG 11	48.29	4.33	-13.51	1.65	147.82	12.08	-412.93	11.70	1.23	0.05	-229.10	4.22
DA 12	46.92	4.27	-11.19	1.56	187.80	11.40	-390.04	11.08	1.31	0.05	-165.21	4.16
DC 13	45.43	4.20	-5.97	1.73	89.03	7.12	-378.80	6.52	1.39	0.06	-248.93	3.97
DA 14	46.66	4.24	-11.52	1.55	166.91	5.82	-369.21	5.38	1.21	0.06	-165.96	4.10
DT 15	48.22	3.98	-8.39	1.65	201.28	4.79	-365.75	4.44	1.52	0.06	-123.11	4.10
DG 16	47.14	4.27	-12.08	1.63	104.46	5.59	-357.47	4.93	1.33	0.05	-216.61	4.16
DC 17	46.10	4.32	-6.47	1.72	48.41	5.49	-339.38	4.66	1.36	0.05	-249.98	4.04
DA 18	46.40	4.26	-11.43	1.54	121.54	5.67	-324.28	5.11	1.22	0.06	-166.54	4.14
DT 19	48.08	3.88	-9.09	1.63	144.96	5.51	-309.70	5.23	1.40	0.07	-124.34	4.01
DT3 20	47.16	3.93	-3.65	1.58	83.99	4.83	-218.40	4.68	2.29	0.07	-88.62	4.01
RA5 21	47.53	4.11	-2.72	1.58	-17.04	6.92	-106.06	6.17	1.89	0.07	-76.40	4.14
RA 22	50.55	4.35	-10.76	1.81	132.71	13.53	-342.29	12.82	1.30	0.06	-168.48	4.43
RU 23	46.52	3.78	-8.34	1.78	173.74	12.22	-364.70	11.72	1.35	0.05	-151.44	4.11
RG 24	51.72	4.40	-13.37	1.83	129.17	14.38	-388.95	13.64	1.34	0.05	-220.09	4.47
RC 25	49.31	4.15	-7.48	1.92	88.05	12.73	-384.58	12.02	1.32	0.05	-253.38	4.21
RA 26	50.59	4.20	-12.09	1.75	190.02	11.84	-398.06	11.23	1.29	0.05	-168.25	4.32
RU 27	46.61	3.79	-8.28	1.78	215.11	10.13	-405.70	9.75	1.35	0.05	-150.91	4.14
RG 28	51.69	4.35	-13.41	1.86	160.00	9.98	-420.00	9.19	1.33	0.05	-220.39	4.50
RU 29	46.60	3.76	-9.07	1.73	220.20	7.86	-409.95	7.39	1.28	0.04	-150.94	4.09
RC 30	48.94	4.16	-6.90	1.85	103.25	7.54	-399.37	6.94	1.36	0.04	-252.73	4.21
RA 31	50.52	4.25	-11.94	1.79	190.37	7.50	-397.99	6.59	1.28	0.05	-167.76	4.36
RC 32	49.11	4.17	-7.14	1.86	93.52	6.93	-388.80	6.14	1.34	0.05	-251.97	4.23
RA 33	50.26	4.23	-11.43	1.79	179.60	7.08	-388.46	6.46	1.35	0.05	-168.69	4.34
RG 34	51.10	4.32	-13.14	1.77	132.77	7.24	-393.41	6.41	1.39	0.05	-221.29	4.35
RG 35	51.33	4.28	-14.32	1.78	126.22	6.70	-386.59	5.84	1.29	0.05	-222.06	4.37
RC 36	49.18	4.15	-7.53	1.93	69.03	5.69	-365.36	4.84	1.33	0.05	-253.35	4.16
RG 37	51.15	4.27	-13.10	1.86	104.56	6.62	-365.23	5.73	1.39	0.06	-221.23	4.38
RG 38	51.07	4.29	-13.86	1.76	93.82	6.44	-355.07	5.56	1.36	0.05	-222.68	4.37
RG 39	50.94	4.21	-13.78	1.79	75.24	6.26	-336.87	5.35	1.33	0.05	-223.14	4.29
RA3 40	49.93	4.26	-5.38	1.76	49.65	5.88	-229.52	5.15	2.24	0.06	-133.08	4.17

Table SIII.16. Total delta per-residue GBSA energy decomposition (kcal/mol) averaged along the 5 ns MD trajectory modeling the ***7′R*-Me-cLNA-T modified at position 11** AON-RNA duplex (AON20). Contributions from 1-4 interactions are added to the electrostatic and van der Waals energy components and Generalized Born approach is utilized to describe solvent contributions.

Residue	**van der Waals**		**Electrostatic**		**Polar Solv.**		**Non-Polar Solv.**		**TOTAL**	
	Avg.	***σ***	***Avg.***	***σ***	***Avg.***	***σ***	***Avg.***	***σ***	***Avg.***	***σ***
DT5 1	-0.78	0.64	36.80	2.48	-37.73	2.25	-0.26	0.02	-1.97	0.48
DC 2	-1.91	0.87	119.54	8.64	-121.97	8.38	-0.32	0.04	-4.67	0.79
DC 3	-2.98	0.92	123.08	7.58	-125.87	7.36	-0.39	0.03	-6.16	0.87
DC 4	-2.97	0.92	129.83	6.30	-132.55	6.09	-0.38	0.03	-6.08	0.84
DG 5	-4.70	1.00	142.31	6.74	-144.05	6.54	-0.56	0.06	-6.99	1.07
DC 6	-1.43	0.89	147.49	6.69	-150.55	6.38	-0.21	0.03	-4.70	0.72
DC 7	-3.04	0.94	148.34	6.44	-151.08	6.18	-0.39	0.04	-6.16	0.85
DT 8	-3.44	0.78	160.02	5.69	-159.17	5.52	-0.35	0.04	-2.94	0.72
DG 9	-4.45	0.97	148.55	6.41	-151.51	6.19	-0.57	0.05	-7.98	0.94
cLNA-T 10	**-2.10**	**0.64**	**166.89**	**6.65**	**-166.14**	**6.45**	**-0.18**	**0.03**	**-1.53**	**0.54**
DG 11	-3.86	0.94	158.47	8.23	-161.58	7.90	-0.48	0.04	-7.46	0.95
DA 12	-3.24	0.74	157.47	8.00	-157.42	7.84	-0.37	0.04	-3.56	0.74
DC 13	-1.20	0.86	140.62	5.80	-143.45	5.44	-0.21	0.04	-4.24	0.76
DA 14	-4.84	0.86	137.93	4.25	-137.57	4.06	-0.55	0.05	-5.04	0.80
DT 15	-1.95	0.68	135.71	3.66	-135.50	3.41	-0.22	0.04	-1.95	0.57
DG 16	-4.28	0.95	120.44	3.80	-122.71	3.42	-0.55	0.05	-7.10	0.94
DC 17	-1.16	0.87	113.67	3.41	-117.35	3.02	-0.18	0.03	-5.02	0.72
DA 18	-4.54	0.85	111.14	3.14	-111.21	2.81	-0.53	0.05	-5.14	0.79
DT 19	-1.90	0.66	109.44	3.40	-109.40	3.11	-0.24	0.04	-2.09	0.59
DT3 20	-2.38	0.71	71.27	2.85	-70.34	2.54	-0.41	0.06	-1.86	0.83
RA5 21	-1.12	0.61	35.19	2.43	-36.06	2.19	-0.29	0.05	-2.29	0.82
RA 22	-2.78	0.74	136.68	7.94	-136.76	7.76	-0.42	0.05	-3.28	0.75
RU 23	-1.62	0.67	145.06	8.13	-145.09	7.85	-0.19	0.03	-1.84	0.56
RG 24	-4.34	0.99	143.80	9.68	-146.22	9.33	-0.55	0.05	-7.32	1.07
RC 25	-1.24	0.87	149.22	8.67	-152.42	8.34	-0.18	0.03	-4.62	0.70
RA 26	-4.48	0.83	157.75	7.94	-157.27	7.66	-0.51	0.04	-4.50	0.88
RU 27	-1.73	0.70	163.84	6.65	-163.56	6.48	-0.20	0.04	-1.65	0.57
RG 28	-4.54	1.03	155.38	6.67	-158.50	6.41	-0.59	0.05	-8.24	1.00
RU 29	-1.89	0.71	168.00	5.85	-167.71	5.60	-0.18	0.03	-1.79	0.63
RC 30	-2.25	0.87	153.21	5.71	-155.04	5.35	-0.30	0.03	-4.39	0.81
RA 31	-4.83	0.79	151.68	5.10	-150.61	4.84	-0.52	0.04	-4.28	0.76
RC 32	-1.37	0.85	137.93	5.10	-140.16	4.74	-0.22	0.03	-3.83	0.75
RA 33	-4.11	0.85	137.90	4.95	-137.89	4.69	-0.46	0.04	-4.55	0.76
RG 34	-3.00	0.95	122.65	4.60	-126.44	4.41	-0.42	0.04	-7.22	0.88
RG 35	-3.76	0.97	121.59	4.31	-125.09	4.01	-0.47	0.04	-7.73	0.97
RC 36	-1.39	0.89	123.66	3.26	-126.80	2.89	-0.21	0.03	-4.73	0.72
RG 37	-3.87	1.07	104.43	3.19	-108.16	3.02	-0.48	0.06	-8.08	1.09
RG 38	-3.04	0.93	98.83	3.60	-103.67	3.47	-0.40	0.04	-8.28	0.89
RG 39	-3.27	0.93	98.78	3.44	-103.11	3.21	-0.41	0.04	-8.01	0.91
RA3 40	-2.52	0.74	73.47	2.72	-73.43	2.56	-0.43	0.04	-2.91	0.60

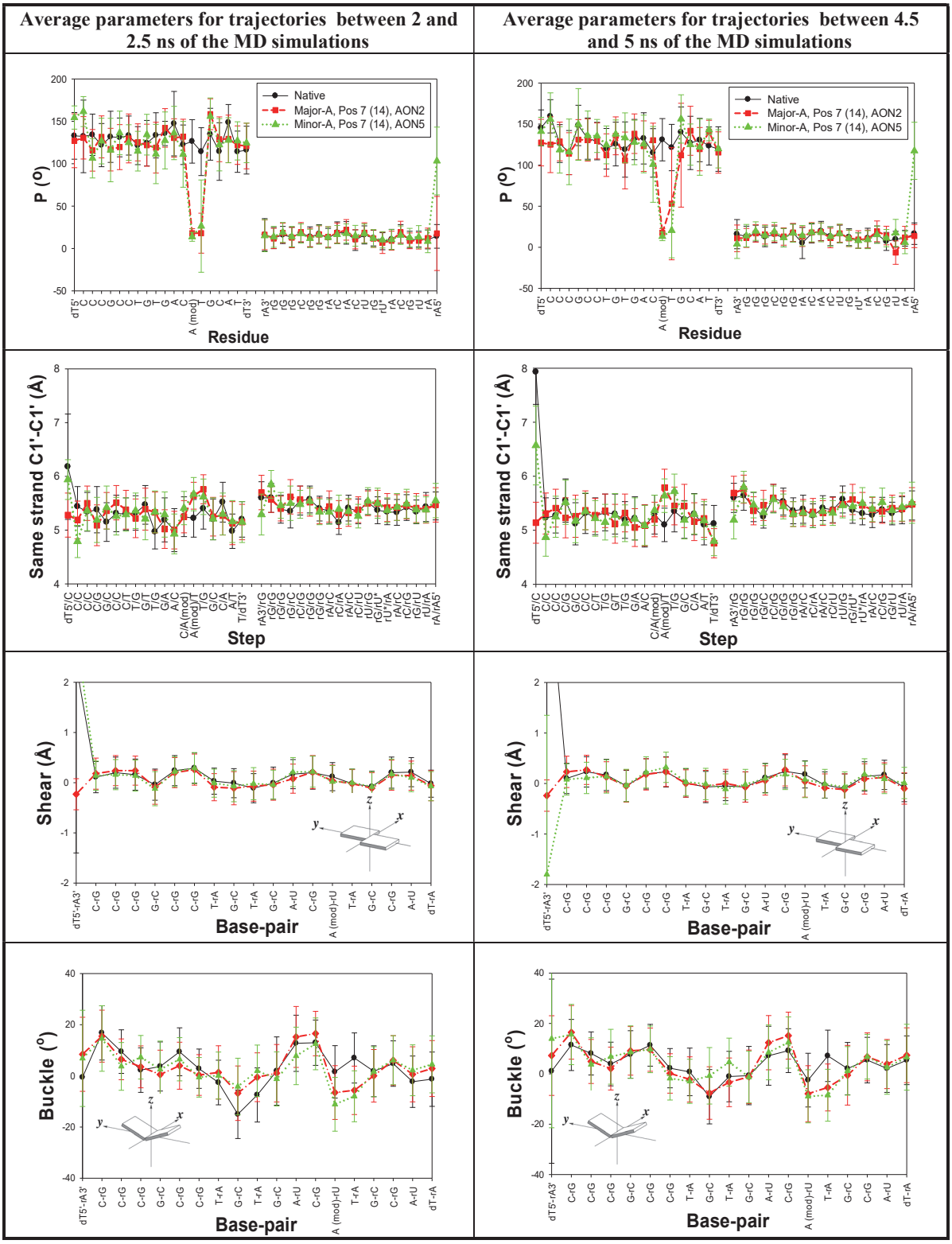
Table SIII.17. Total per-residue GBSA energy decomposition (kcal/mol) averaged along the 5 ns MD trajectory modeling the ***7′S*-Me-cLNA-T modified at position 11** AON-RNA duplex (AON23). Contributions from 1-4 interactions are added to the electrostatic and van der Waals energy components and Generalized Born approach is utilized to describe solvent contributions.

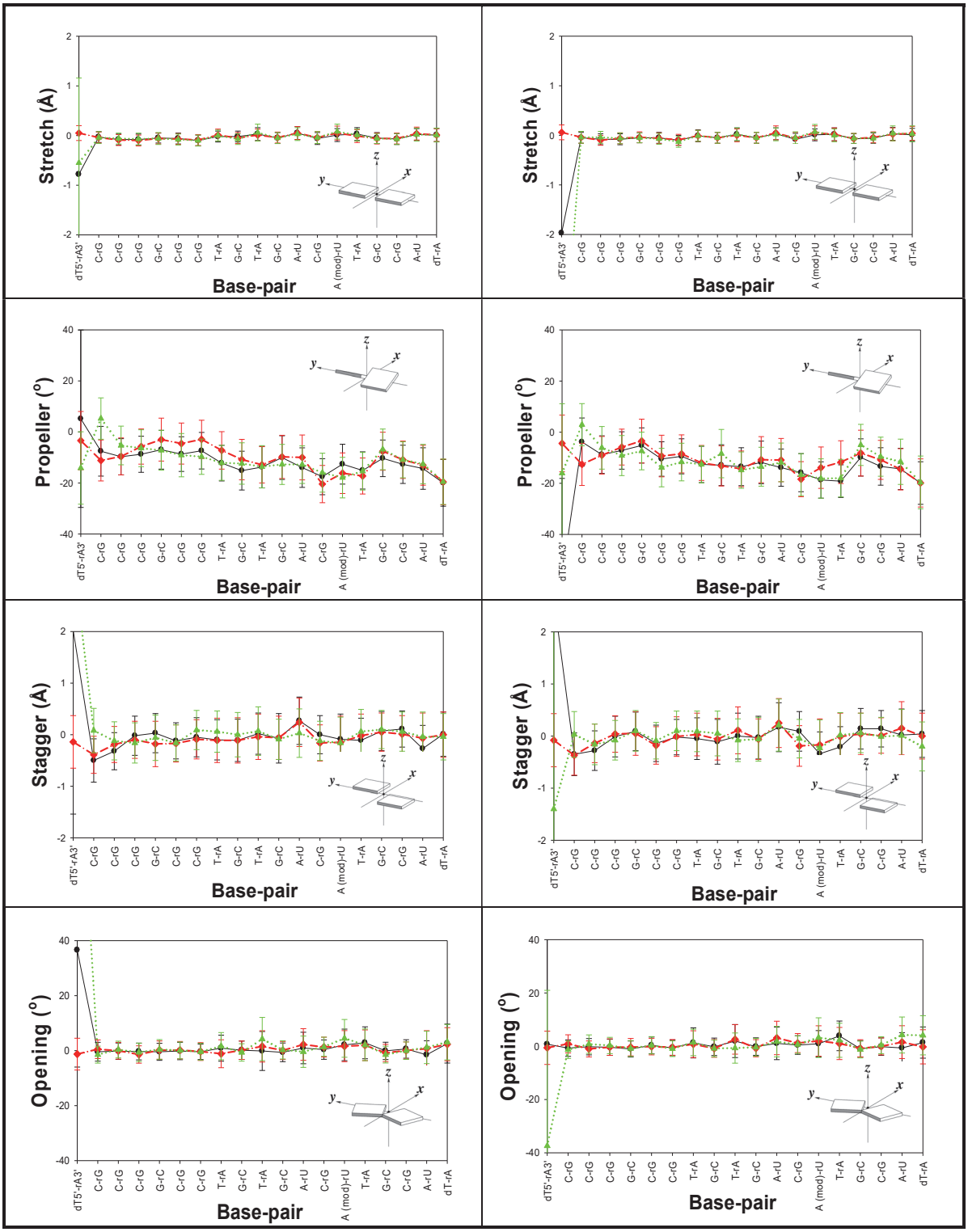
Residue	**Internal**		**van der Waals**		**Electrostatic**		**Polar Solv.**		**Non-Polar Solv.**		**TOTAL**	
	Avg.	***σ***	***Avg.***	***σ***	***Avg.***	***σ***	***Avg.***	***σ***	***Avg.***	***σ***	***Avg.***	***σ***
DT5 1	42.63	3.95	-0.56	2.23	11.20	5.07	-98.88	5.35	1.91	0.14	-43.69	3.87
DC 2	47.89	4.40	-4.90	1.87	17.99	9.63	-308.52	9.02	1.36	0.07	-246.19	4.10
DC 3	45.90	4.23	-6.29	1.69	51.04	9.32	-341.66	8.95	1.30	0.06	-249.70	4.02
DC 4	45.87	4.23	-6.35	1.75	69.19	8.80	-359.84	8.46	1.33	0.06	-249.80	4.05
DG 5	47.51	4.32	-12.28	1.64	122.66	9.61	-375.82	9.15	1.34	0.05	-216.59	4.19
DC 6	45.65	4.21	-6.40	1.70	90.42	10.08	-380.11	9.61	1.35	0.05	-249.09	4.03
DC 7	45.56	4.15	-7.25	1.67	96.54	10.07	-386.15	9.67	1.24	0.05	-250.06	3.92
DT 8	48.27	3.97	-9.31	1.65	227.79	9.90	-391.72	9.62	1.42	0.06	-123.55	4.08
DG 9	47.63	4.37	-12.62	1.73	142.14	11.70	-395.30	11.25	1.30	0.05	-216.85	4.29
cLNA-T 10	**77.61**	**4.73**	**-2.97**	**2.32**	**-22.14**	**8.90**	**-384.38**	**8.22**	**1.83**	**0.04**	**-330.05**	**4.56**
DG 11	48.71	4.34	-13.38	1.71	144.13	11.42	-410.70	10.83	1.18	0.05	-230.05	4.35
DA 12	47.09	4.40	-11.25	1.54	187.09	9.88	-389.35	9.41	1.29	0.06	-165.13	4.29
DC 13	45.41	4.23	-5.89	1.74	86.08	7.18	-376.03	6.51	1.39	0.06	-249.05	4.00
DA 14	46.39	4.26	-11.48	1.54	163.74	5.78	-366.05	5.29	1.21	0.06	-166.18	4.13
DT 15	48.44	4.06	-8.37	1.69	198.07	4.99	-362.63	4.64	1.53	0.06	-122.96	4.22
DG 16	47.33	4.31	-12.05	1.63	101.99	5.86	-355.27	5.18	1.34	0.05	-216.67	4.16
DC 17	45.88	4.23	-6.48	1.72	49.20	6.25	-340.01	5.56	1.36	0.05	-250.05	4.00
DA 18	46.30	4.18	-11.36	1.53	122.65	6.26	-325.33	5.71	1.22	0.06	-166.51	4.08
DT 19	48.28	3.92	-9.01	1.64	145.61	5.54	-310.40	5.31	1.41	0.07	-124.11	4.06
DT3 20	47.29	4.03	-3.53	1.60	84.10	4.74	-218.62	4.47	2.29	0.06	-88.47	4.16
RA5 21	47.14	4.04	-2.73	1.55	-17.86	6.49	-105.35	5.91	1.88	0.05	-76.92	3.91
RA 22	50.44	4.23	-10.72	1.76	130.40	13.77	-340.17	13.01	1.31	0.06	-168.74	4.35
RU 23	46.58	3.80	-8.27	1.76	171.69	11.03	-362.76	10.60	1.35	0.05	-151.40	4.15
RG 24	51.50	4.30	-13.30	1.83	128.25	11.90	-388.34	11.30	1.34	0.05	-220.55	4.39
RC 25	49.27	4.14	-7.45	1.90	89.79	12.70	-386.26	11.85	1.33	0.05	-253.33	4.25
RA 26	50.67	4.21	-12.03	1.74	191.38	13.10	-399.36	12.53	1.29	0.06	-168.06	4.35
RU 27	46.71	3.85	-8.22	1.80	214.30	12.13	-404.98	11.85	1.36	0.05	-150.83	4.20
RG 28	51.51	4.32	-13.34	1.85	157.75	12.76	-417.73	11.82	1.34	0.06	-220.46	4.47
RU 29	46.69	3.77	-8.99	1.75	216.26	9.62	-406.11	9.13	1.29	0.05	-150.85	4.09
RC 30	49.31	4.28	-6.63	1.90	100.33	7.42	-396.61	6.68	1.36	0.05	-252.25	4.50
RA 31	50.58	4.30	-11.88	1.82	189.30	7.53	-396.96	6.56	1.28	0.06	-167.69	4.43
RC 32	49.13	4.15	-7.03	1.85	92.28	6.65	-387.85	5.96	1.34	0.05	-252.13	4.18
RA 33	50.26	4.24	-11.14	1.81	177.82	6.64	-386.70	5.97	1.36	0.05	-168.40	4.36
RG 34	51.16	4.26	-13.07	1.80	131.43	7.24	-392.29	6.52	1.39	0.05	-221.38	4.38
RG 35	51.47	4.30	-14.34	1.77	125.24	6.86	-385.56	5.97	1.29	0.05	-221.89	4.42
RC 36	49.06	4.13	-7.48	1.91	69.77	5.98	-365.89	5.19	1.33	0.05	-253.20	4.20
RG 37	50.94	4.27	-13.13	1.87	105.82	6.92	-366.62	6.12	1.39	0.06	-221.59	4.37
RG 38	51.22	4.23	-13.86	1.78	94.58	6.67	-355.70	5.76	1.36	0.05	-222.40	4.34
RG 39	51.21	4.26	-13.86	1.91	74.79	6.76	-336.18	5.83	1.33	0.06	-222.71	4.44
RA3 40	49.98	4.34	-6.10	2.09	52.40	6.39	-230.27	5.40	2.19	0.15	-131.80	4.31

Table SIII.18. Total delta per-residue GBSA energy decomposition (kcal/mol) averaged along the 5 ns MD trajectory modeling the ***7′S*-Me-cLNA-T** modified at position 11 AON-RNA duplex (AON23). Contributions from 1-4 interactions are added to the electrostatic and van der Waals energy components and Generalized Born approach is utilized to describe solvent contributions.

Residue	**van der Waals**		**Electrostatic**		**Polar Solv.**		**Non-Polar Solv.**		**TOTAL**	
	Avg.	***σ***	***Avg.***	***σ***	***Avg.***		***Avg.***	***σ***	***Avg.***	***σ***
DT5 1	-1.76	1.28	36.54	2.47	-35.93	2.59	-0.26	0.10	-1.40	1.00
DC 2	-1.76	0.87	110.35	7.30	-112.68	7.06	-0.33	0.07	-4.42	0.90
DC 3	-2.87	0.93	122.16	6.66	-124.99	6.46	-0.38	0.04	-6.09	0.88
DC 4	-2.85	0.95	130.29	6.29	-133.07	6.10	-0.37	0.04	-6.00	0.85
DG 5	-4.78	1.01	142.73	6.83	-144.58	6.60	-0.57	0.06	-7.21	1.06
DC 6	-1.49	0.89	148.12	7.28	-151.08	7.02	-0.21	0.03	-4.67	0.72
DC 7	-3.08	0.94	148.34	7.08	-151.02	6.87	-0.40	0.03	-6.15	0.85
DT 8	-3.48	0.78	159.83	7.13	-158.99	6.92	-0.35	0.04	-2.99	0.75
DG 9	-4.33	1.00	148.87	8.20	-151.53	7.94	-0.56	0.05	-7.54	0.99
cLNA-T 10	**-1.86**	**0.68**	**160.63**	**6.38**	**-159.96**	**6.11**	**-0.17**	**0.03**	**-1.37**	**0.56**
DG 11	-4.12	0.99	160.29	7.98	-163.32	7.69	-0.51	0.05	-7.67	0.96
DA 12	-3.40	0.75	156.95	6.53	-156.84	6.36	-0.38	0.04	-3.67	0.77
DC 13	-1.19	0.86	138.50	5.45	-141.47	5.06	-0.21	0.04	-4.37	0.75
DA 14	-4.62	0.90	136.09	4.12	-135.87	3.90	-0.53	0.05	-4.94	0.81
DT 15	-1.86	0.68	133.84	3.61	-133.76	3.35	-0.21	0.04	-1.98	0.57
DG 16	-4.23	0.96	119.19	3.97	-121.68	3.61	-0.55	0.05	-7.27	0.93
DC 17	-1.22	0.87	114.50	3.64	-118.02	3.28	-0.19	0.03	-4.93	0.74
DA 18	-4.61	0.84	112.03	3.26	-112.06	2.97	-0.53	0.05	-5.18	0.80
DT 19	-1.92	0.67	109.64	3.22	-109.63	2.97	-0.24	0.04	-2.14	0.57
DT3 20	-2.43	0.72	71.11	2.62	-70.32	2.36	-0.42	0.05	-2.06	0.66
RA5 21	-1.14	0.62	34.49	2.63	-35.51	2.35	-0.30	0.03	-2.45	0.60
RA 22	-2.79	0.75	134.83	8.43	-135.04	8.15	-0.41	0.05	-3.41	0.72
RU 23	-1.60	0.67	143.54	6.91	-143.61	6.71	-0.19	0.04	-1.86	0.56
RG 24	-4.31	1.01	142.83	8.08	-145.49	7.77	-0.55	0.05	-7.52	1.00
RC 25	-1.31	0.89	150.14	8.42	-153.16	8.05	-0.19	0.03	-4.51	0.74
RA 26	-4.60	0.84	158.53	8.82	-157.84	8.53	-0.52	0.05	-4.43	0.91
RU 27	-1.71	0.70	163.13	8.25	-162.90	8.08	-0.20	0.04	-1.67	0.58
RG 28	-4.33	1.03	152.91	8.14	-156.11	7.85	-0.57	0.05	-8.10	1.01
RU 29	-1.80	0.71	164.48	6.43	-164.30	6.19	-0.18	0.03	-1.79	0.64
RC 30	-2.26	0.88	150.64	4.92	-152.51	4.60	-0.31	0.04	-4.45	0.84
RA 31	-5.08	0.88	149.48	4.90	-148.69	4.55	-0.54	0.05	-4.84	0.78
RC 32	-1.40	0.84	136.14	4.50	-138.46	4.17	-0.22	0.04	-3.93	0.72
RA 33	-3.89	0.92	135.78	4.06	-135.89	3.77	-0.44	0.05	-4.43	0.80
RG 34	-2.97	0.97	121.04	4.35	-125.01	4.17	-0.43	0.04	-7.37	0.92
RG 35	-3.74	0.96	120.25	4.34	-123.91	4.06	-0.47	0.04	-7.87	0.94
RC 36	-1.45	0.88	123.65	3.51	-126.62	3.13	-0.21	0.03	-4.62	0.84
RG 37	-4.06	1.08	104.83	3.30	-108.50	3.12	-0.50	0.06	-8.22	1.08
RG 38	-3.04	0.94	99.46	3.45	-104.15	3.27	-0.39	0.04	-8.12	0.98
RG 39	-3.27	0.95	98.18	3.55	-102.31	3.29	-0.41	0.05	-7.81	1.06
RA3 40	-3.14	1.23	75.65	3.40	-73.74	2.88	-0.47	0.14	-1.70	1.26

Figure SIII.3. Geometrical parameters of the native (black circles) and 7′(R/S)-Me-cLNA-A modified AON-RNA duplexes [position 7 modification, AON2 for R- (red squares) and AON5 for S- (green triangles) isomers, respectively]. Average values of the pseudorotational phase angle, same strand C1'-C1' distances, local base-pair, local base-pair step and local base pair helical parameters are shown for two 0.5 ns stretches of the corresponding Amber 12[1] MD trajectories (between 2 and 2.5 ns and 4.5 and 5 ns) using individual snapshots (2500 structures per 0.5 ns) analyzed by 3DNA.[2]

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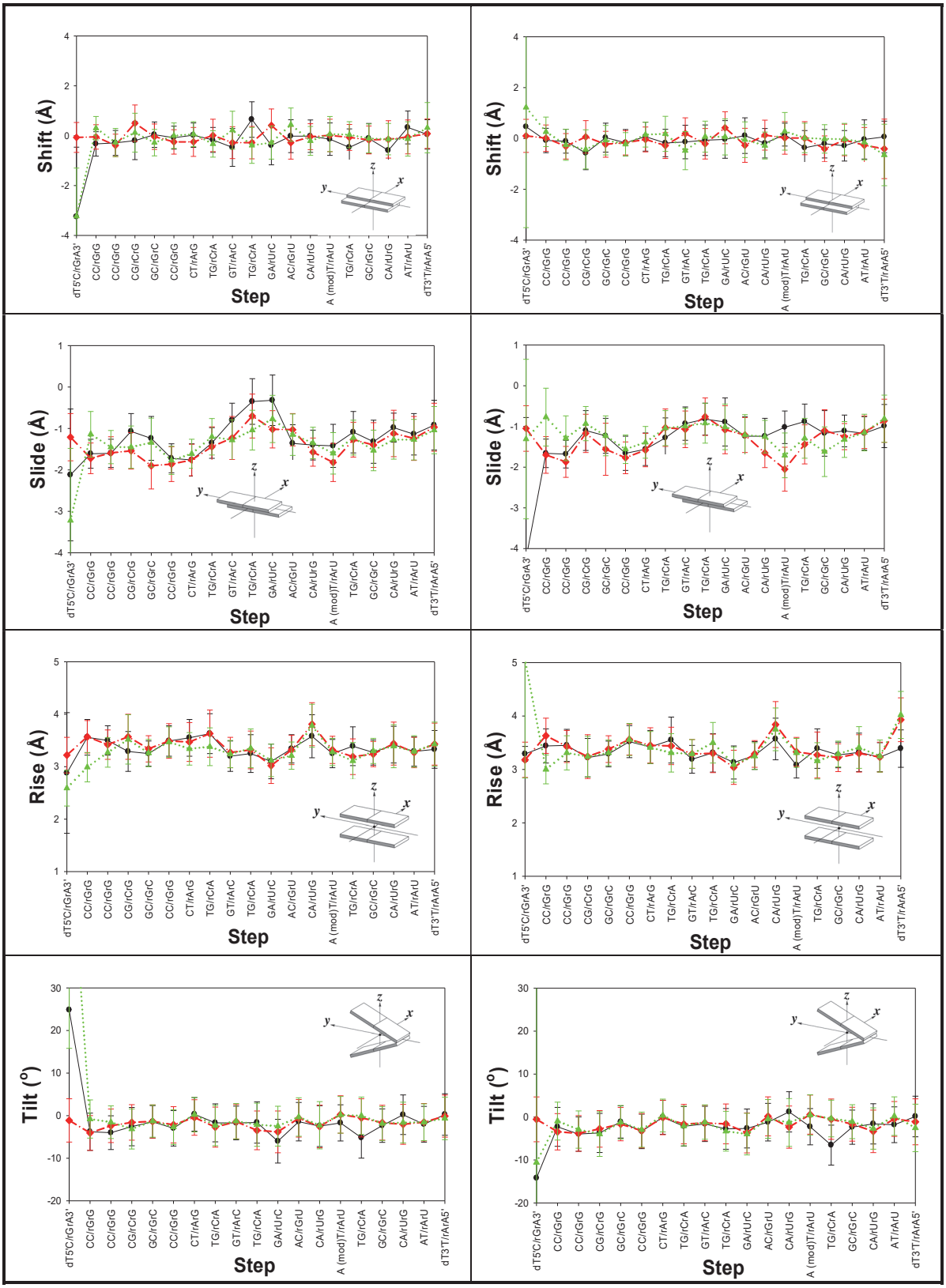
Propeller (°)
Stagger (Å)
Opening (°)
Base-pair
dT5'-rA3'
C-rG
G-rC
T-rA
A-rU
A (mod)-rU
dT-rA
x
y
z


Shift (Å)
Slide (Å)
Rise (Å)
Tilt (°)
Step
dT5'C/rGrA3'
CC/rGrG
CC/rGrG
CG/rCrG
GC/rGrC
CC/rGrG
CT/rArG
TG/rCrA
GT/rArC
TG/rCrA
GA/rUrC
AC/rGrU
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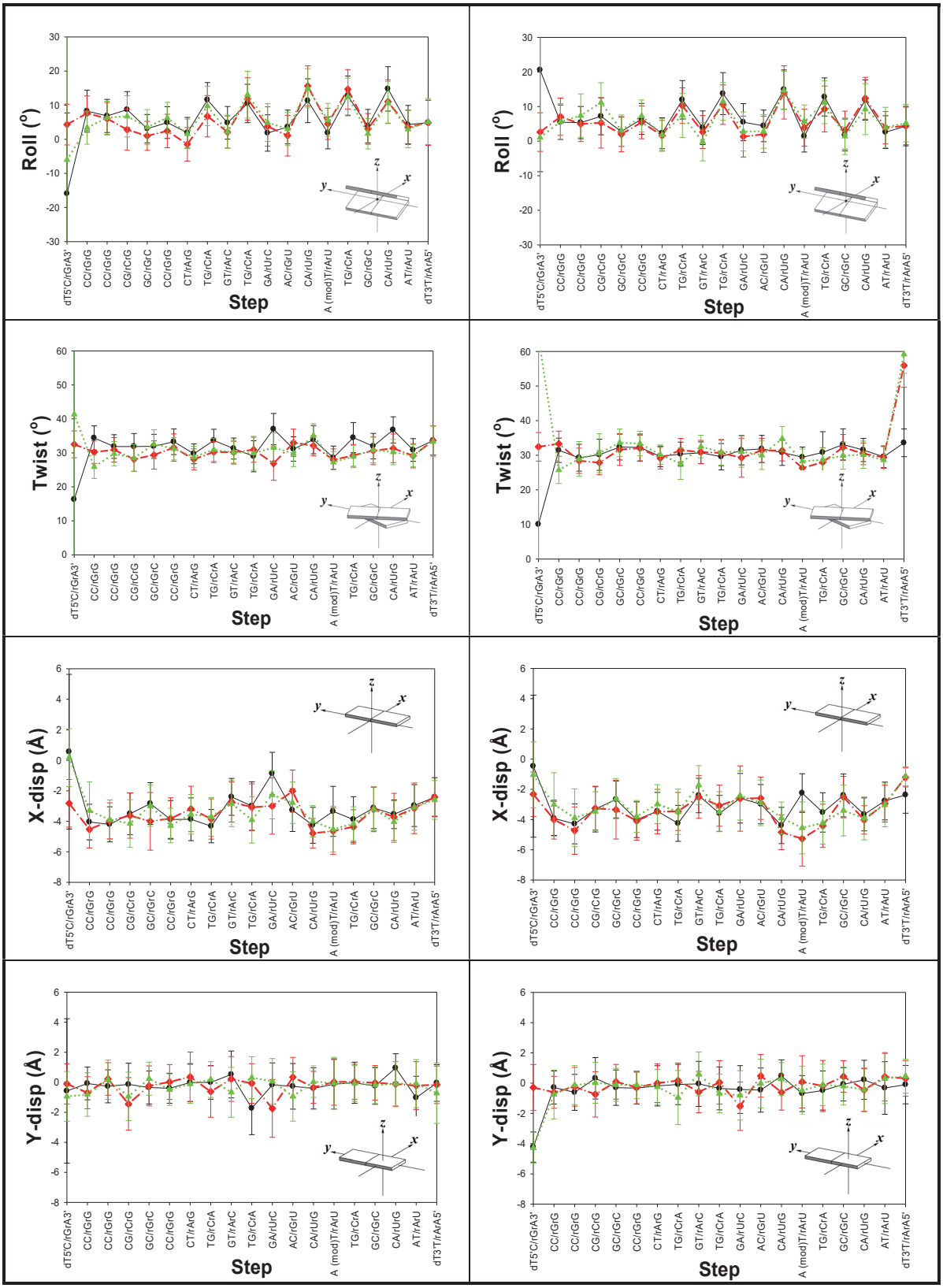
CA/rUrG
AT/rArU
dT3'T/rArA5'


Roll (°)
Twist (°)
X-disp (Å)
Y-disp (Å)
Step
dT5'C/rGrA3'
CC/rGrG
CC/rGrG
CG/rCrG
GC/rGrC
CC/rGrG
CT/rArG
TG/rCrA
GT/rArC
TG/rCrA
GA/rUrC
AC/rGrU
CA/rUrG
A (mod)T/rArU
TG/rCrA
GC/rGrC
CA/rUrG
AT/rArU
dT3'T/rArA5'
z
y
x

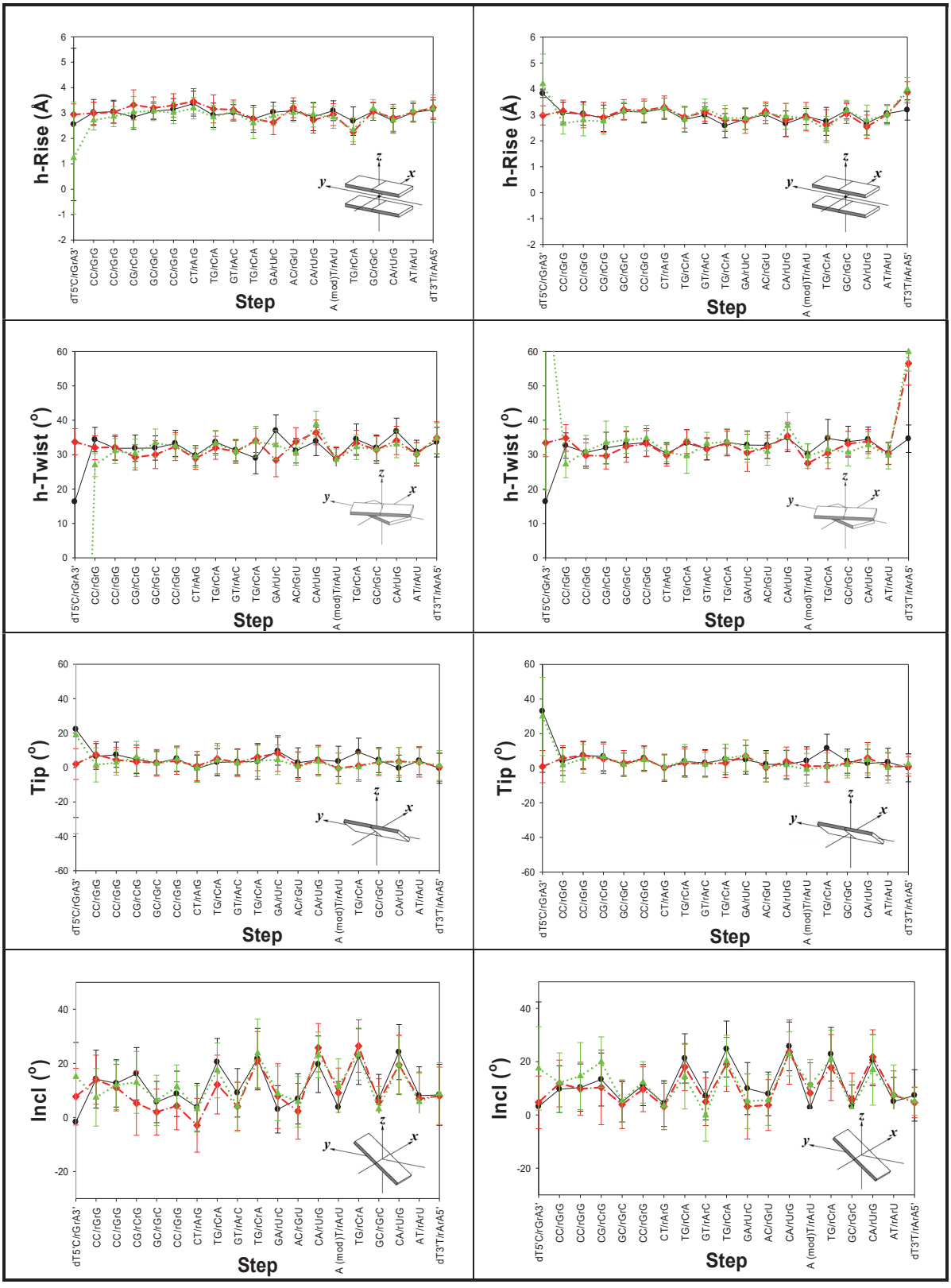
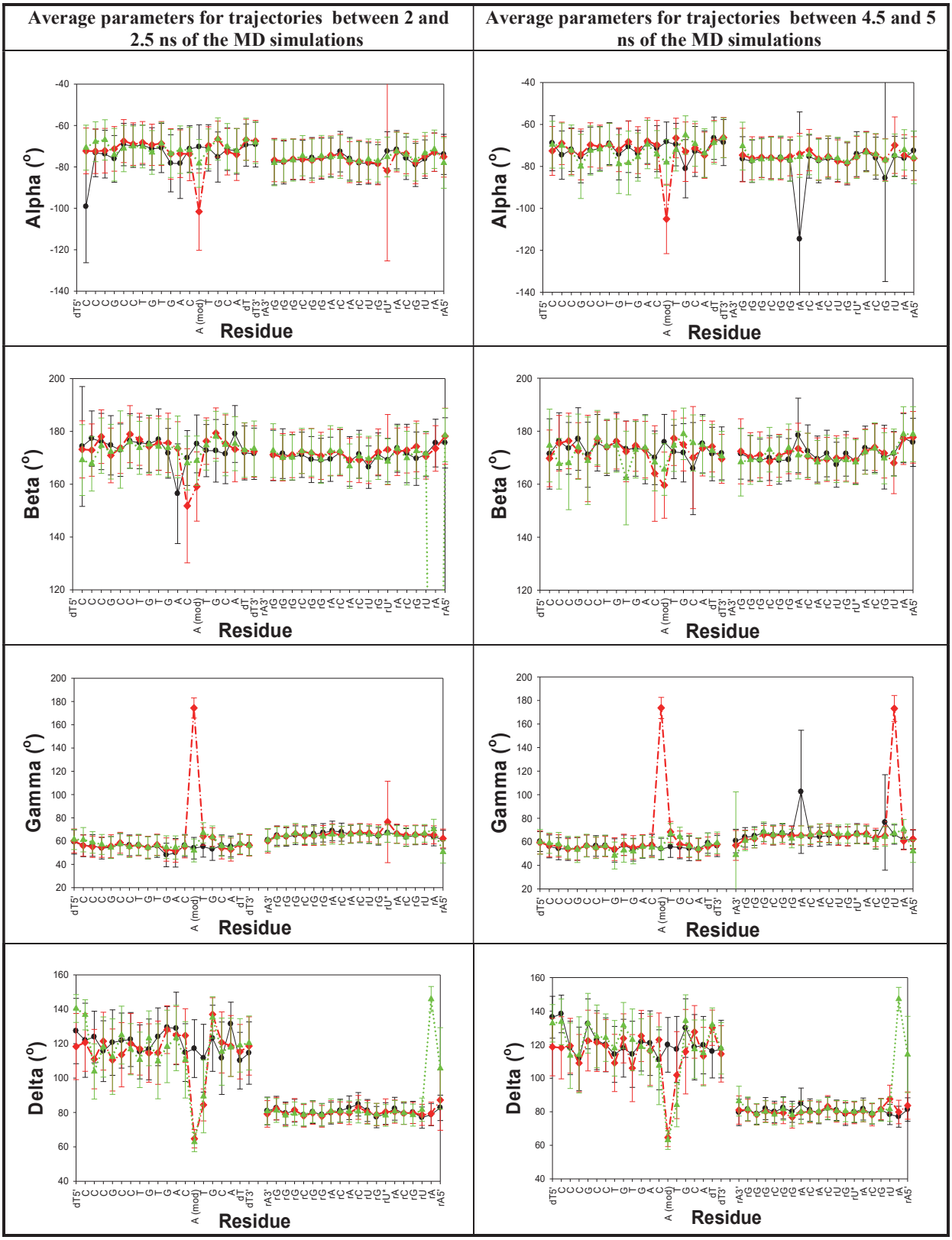

h-Rise (Å)
h-Twist (°)
Tip (°)
Incl (°)
Step
dT5'C/rGrA3'
CC/rGrG
CC/rGrG
CG/rCrG
GC/rGrC
CC/rGrG
CT/rArG
TG/rCrA
GT/rArC
TG/rCrA
GA/rUrC
AC/rGrU
CA/rUrG
A (mod)T/rArU
TG/rCrA
GC/rGrC
CA/rUrG
AT/rArU
dT3'T/rArA5'
x
y
z

Figure SIII.4. Major endocyclic torsions (α, β, γ, δ, ε, ζ, χ)[3] of the native (black circles) and 7′(R/S)-Me-cLNA-A modified AON-RNA duplexes [position 7 modification, AON2 for R- (red squares) and AON5 for S- (green triangles) isomers, respectively] obtained using Amber 12[1] MD trajectories. Average values are shown for two 0.5 ns stretches of the MD trajectories between 2 and 2.5 ns and 4.5 and 5 ns using individual snapshots (2500 structures per 0.5 ns) analyzed by 3DNA.[2]



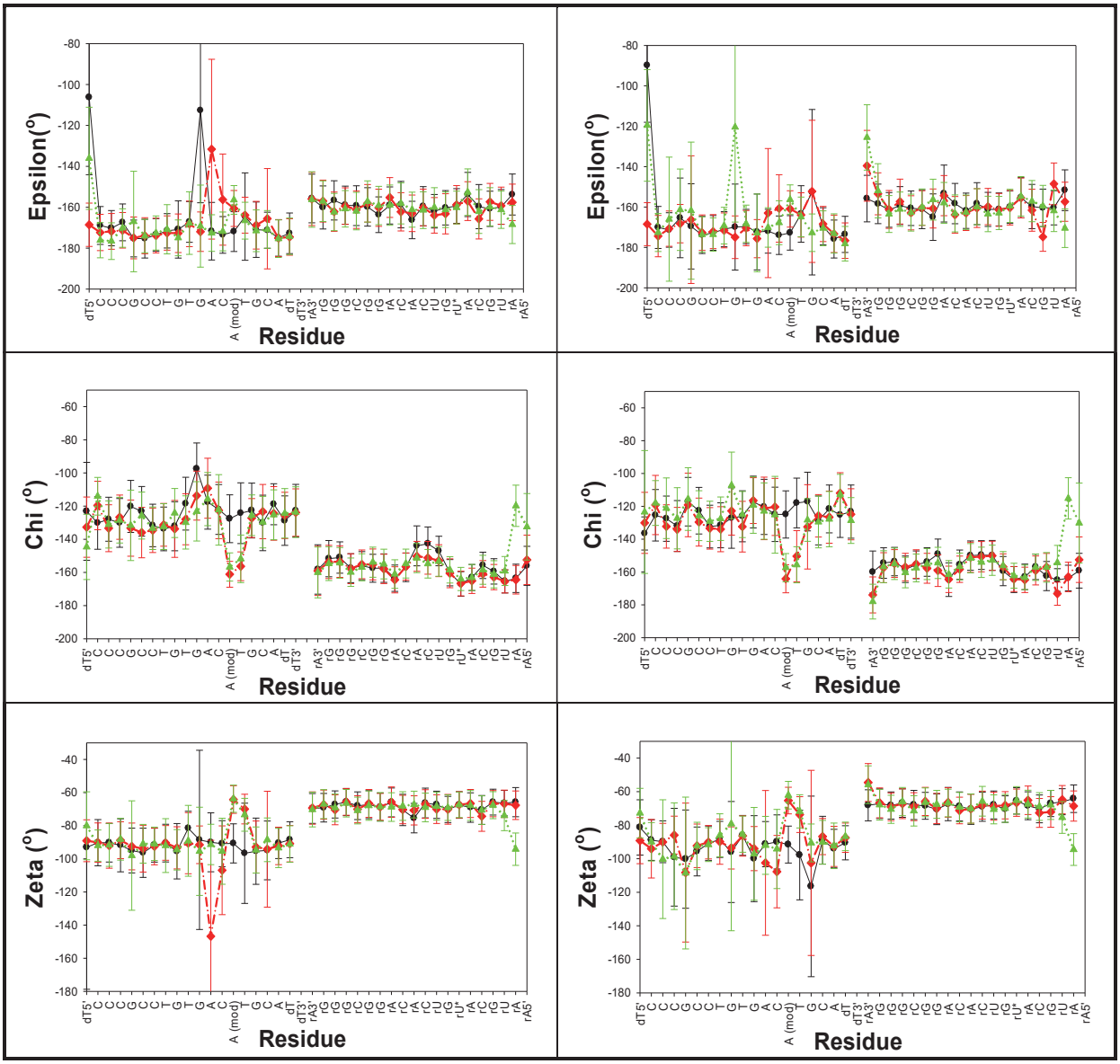
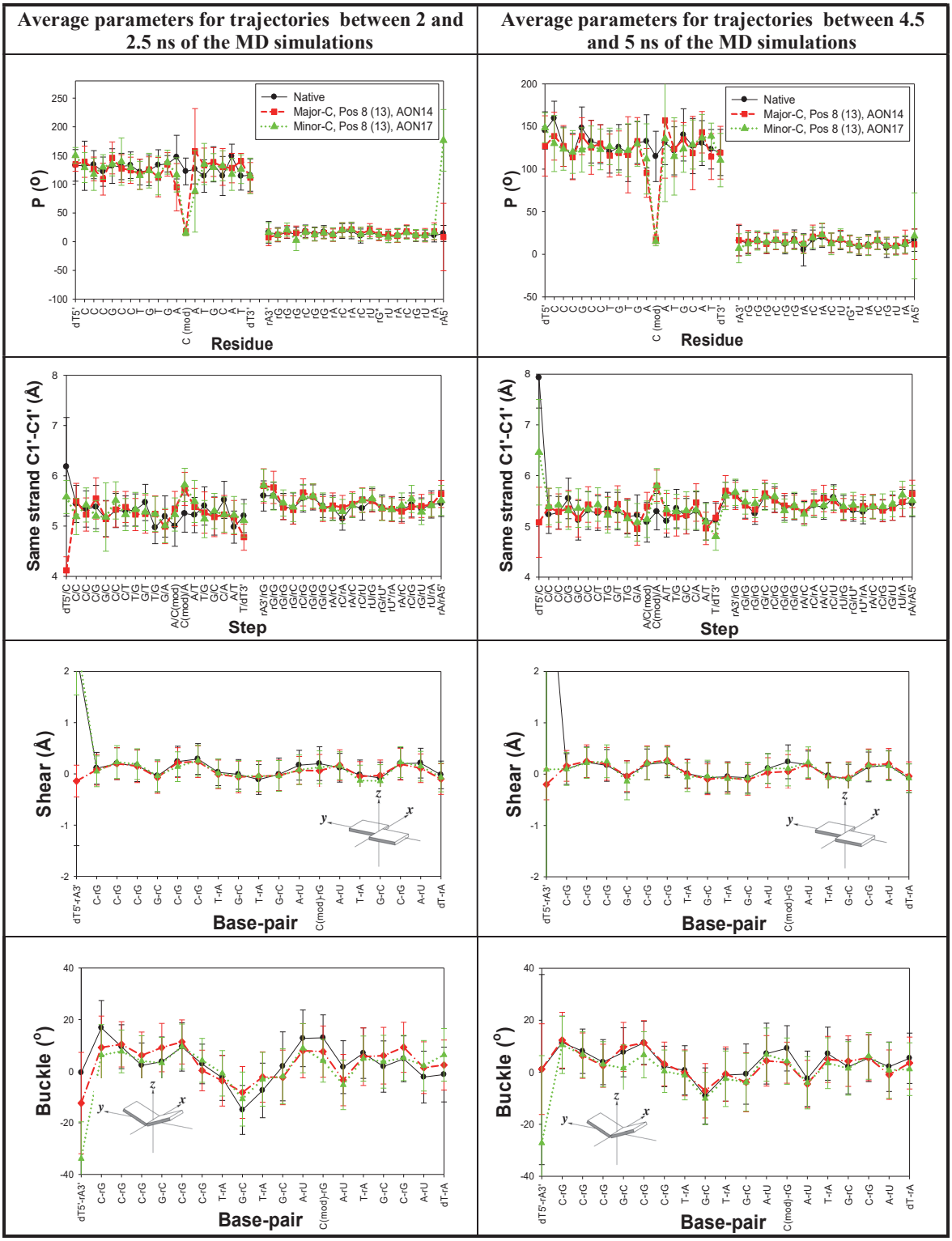
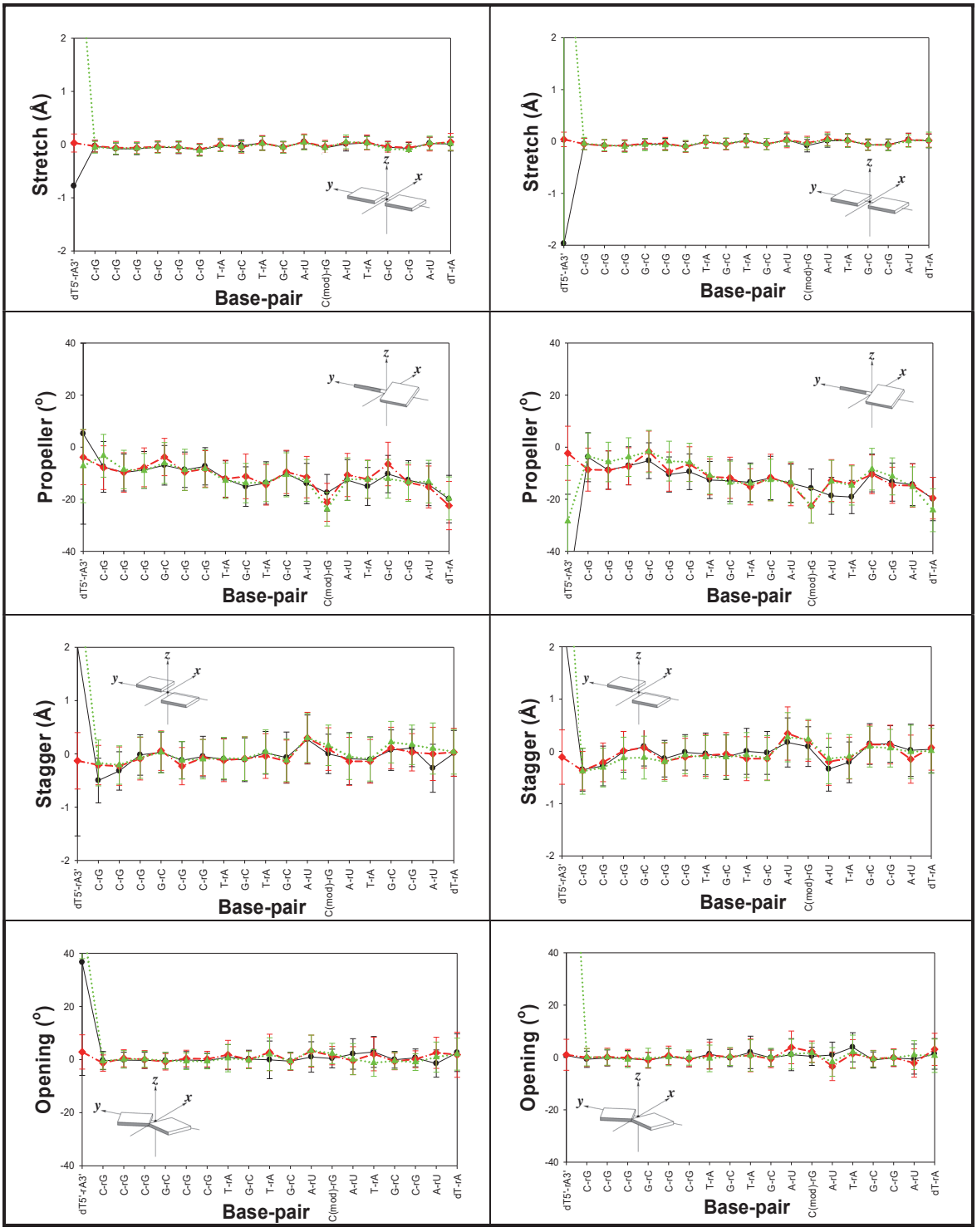
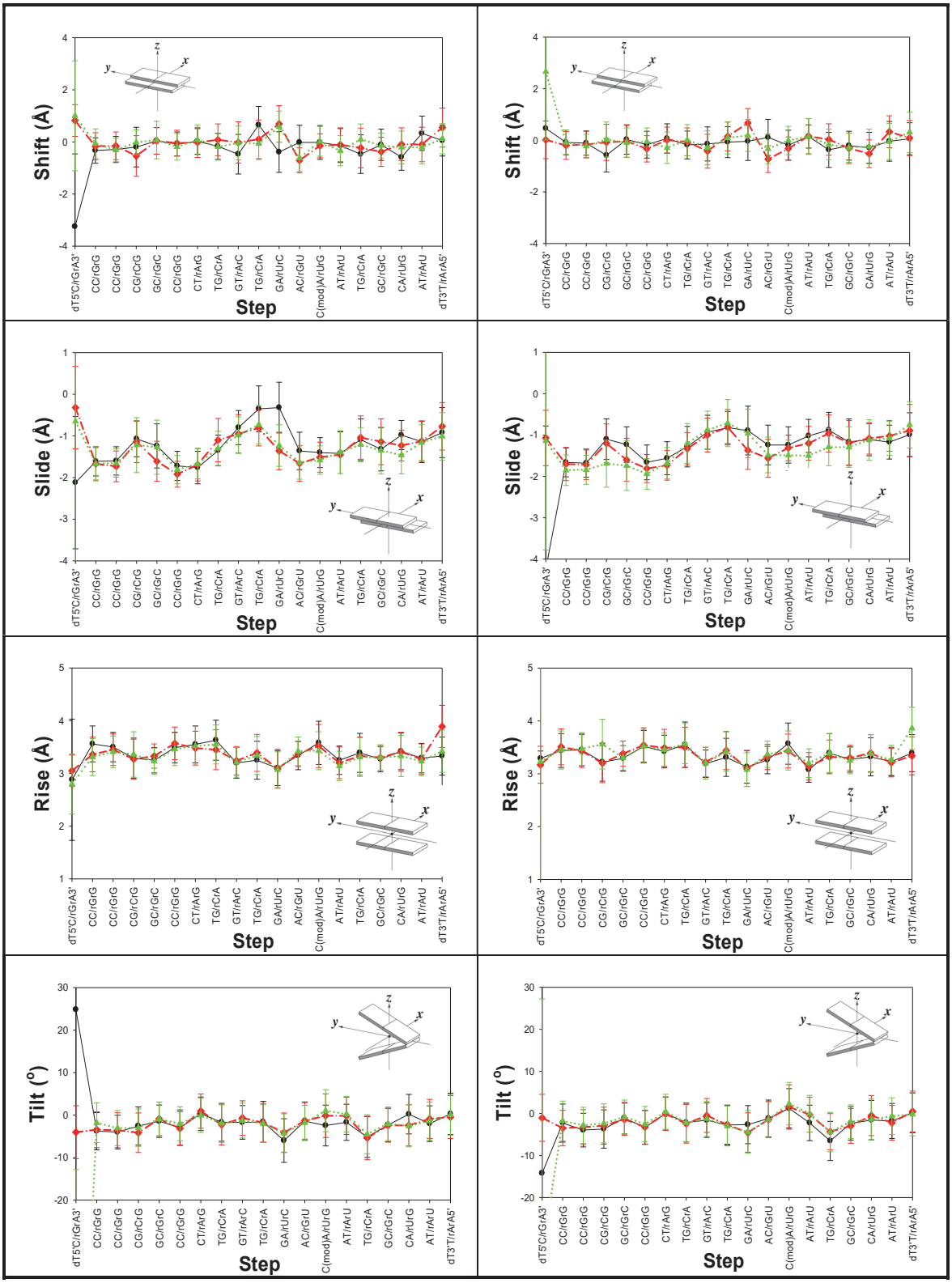

Epsilon(°)
Chi (°)
Zeta (°)
Residue

Figure SIII.5. Geometrical parameters of the native (black circles) and 7′(R/S)-Me-cLNA-^{Me}C modified AON-RNA duplexes [position 8 modification, AON14 for R- (red squares) and AON17 for S- (green triangles) isomers, respectively]. Average values of the pseudorotational phase angle, same strand C1'-C1' distances, local base-pair, local base-pair step and local base pair helical parameters are shown for two 0.5 ns stretches of the corresponding Amber 12[1] MD trajectories (between 2 and 2.5 ns and 4.5 and 5 ns) using individual snapshots (2500 structures per 0.5 ns) analyzed by 3DNA.[2]




Stretch (Å)
Propeller (°)
Stagger (Å)
Opening (°)
Base-pair
dT5'-rA3'
C-rG
C-rG
C-rG
G-rC
C-rG
C-rG
T-rA
G-rC
T-rA
G-rC
A-rU
C(mod)-rG
A-rU
T-rA
G-rC
C-rG
A-rU
dT-rA
z
y
x


Shift (Å)
Slide (Å)
Rise (Å)
Tilt (°)
Step
dT5'C/rGrA3'
CC/rGrG
CC/rGrG
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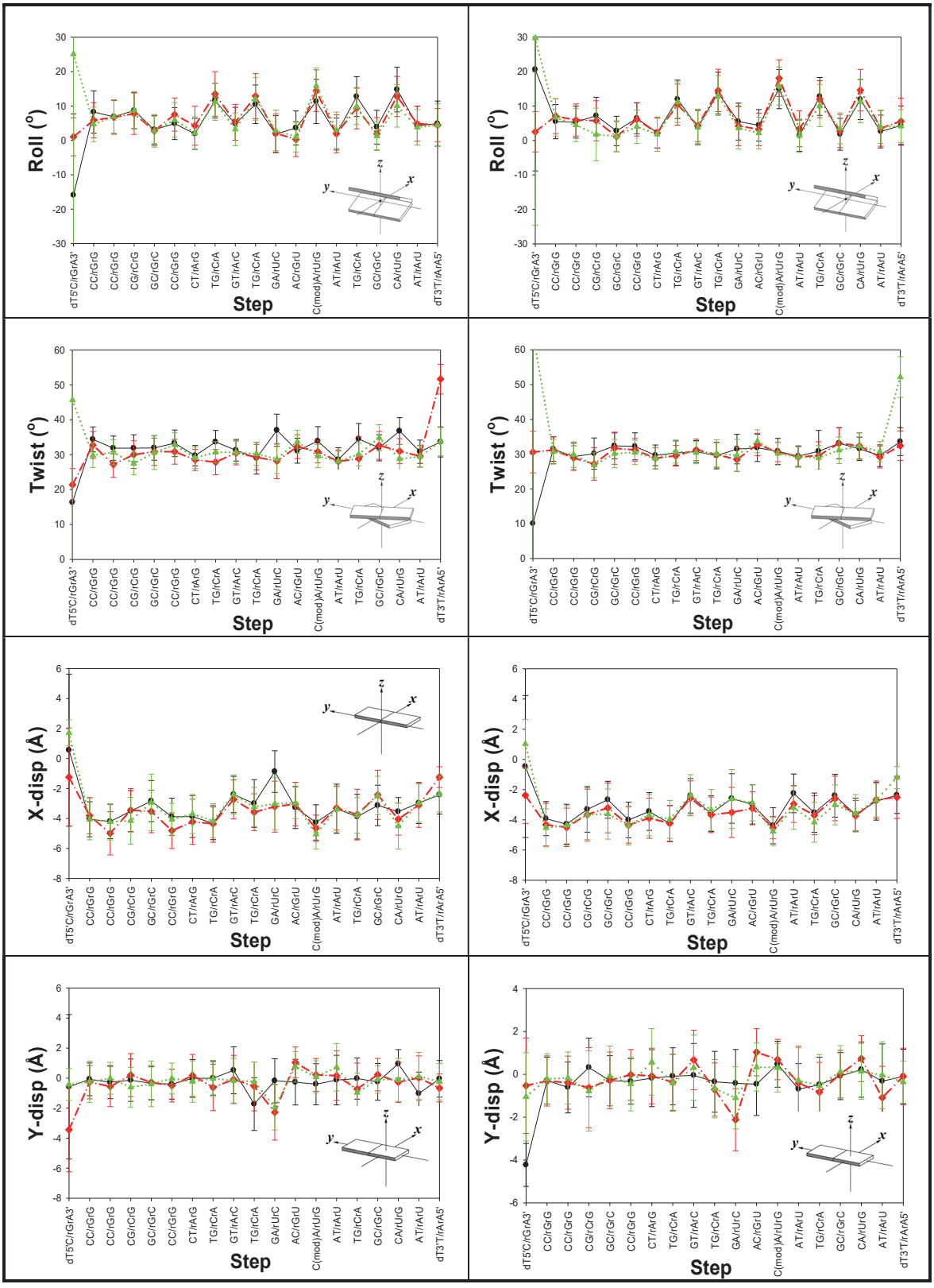
GC/rGrC
CC/rGrG
CT/rArG
TG/rCrA
GT/rArC
TG/rCrA
GA/rUrC
AC/rGrU
C(mod)A/rUrG
AT/rArU
TG/rCrA
GC/rGrC
CA/rUrG
AT/rArU
dT3'T/rArA5'


Roll (°)
Twist (°)
X-disp (Å)
Y-disp (Å)
Step
dT5'C/rGrA3'
CC/rGrG
CC/rGrG
CG/rCrG
GC/rGrC
CC/rGrG
CT/rArG
TG/rCrA
GT/rArC
TG/rCrA
GA/rUrC
AC/rGrU
C(mod)A/rUrG
AT/rArU
TG/rCrA
GC/rGrC
CA/rUrG
AT/rArU
dT3'T/rArA5'
z
x
y

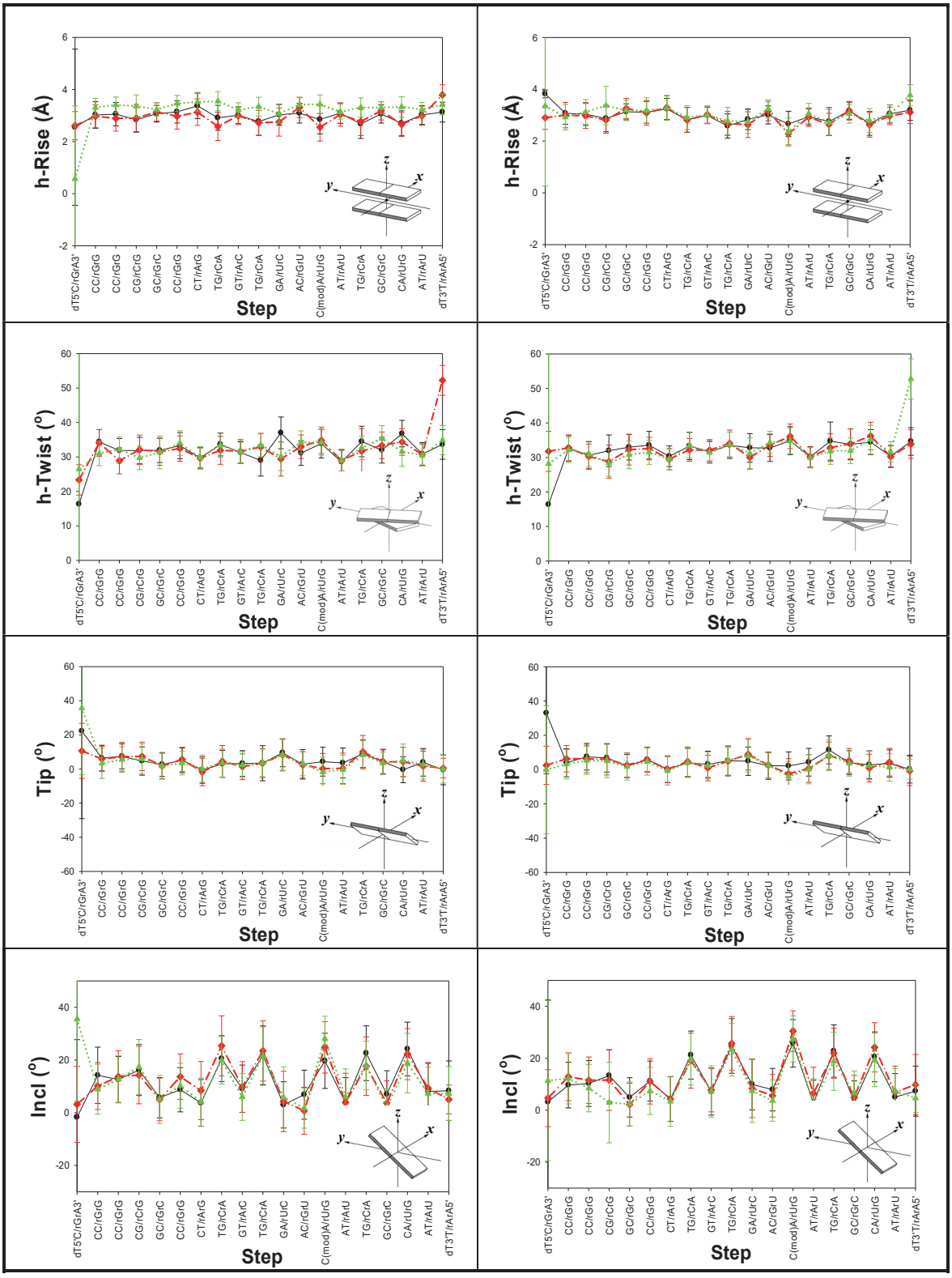
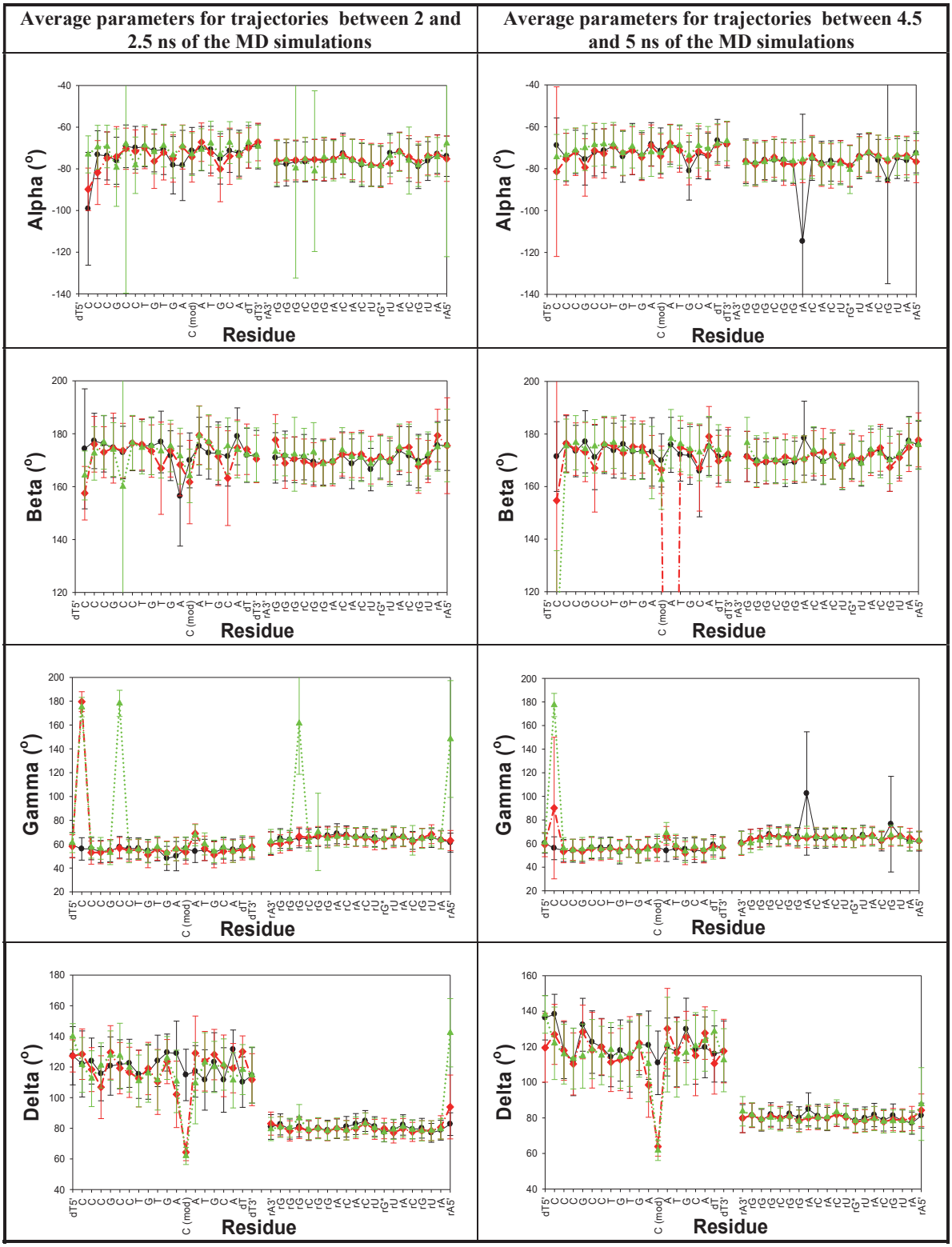

h-Rise (Å)
h-Twist (°)
Tip (°)
Incl (°)
Step
dT5'C/rGrA3'
CC/rGrG
CC/rGrG
CG/rCrG
GC/rGrC
CC/rGrG
CT/rArG
TG/rCrA
GT/rArC
TG/rCrA
GA/rUrC
AC/rGrU
C(mod)A/rUrG
AT/rArU
TG/rCrA
GC/rGrC
CA/rUrG
AT/rArU
dT3'T/rArA5'

Figure SIII.6. Major endocyclic torsions (α, β, γ, δ, ε, ζ, χ)[3] of the native (black circles) and 7′(R/S)-Me-cLNA-^{Me}C modified AON-RNA duplexes [position 8 modification, AON14 for R- (red squares) and AON17 for S- (green triangles) isomers, respectively] obtained using Amber 12[1] MD trajectories. Average values are shown for two 0.5 ns stretches of the MD trajectories between 2 and 2.5 ns and 4.5 and 5 ns using individual snapshots (2500 structures per 0.5 ns) analyzed by 3DNA.[2]



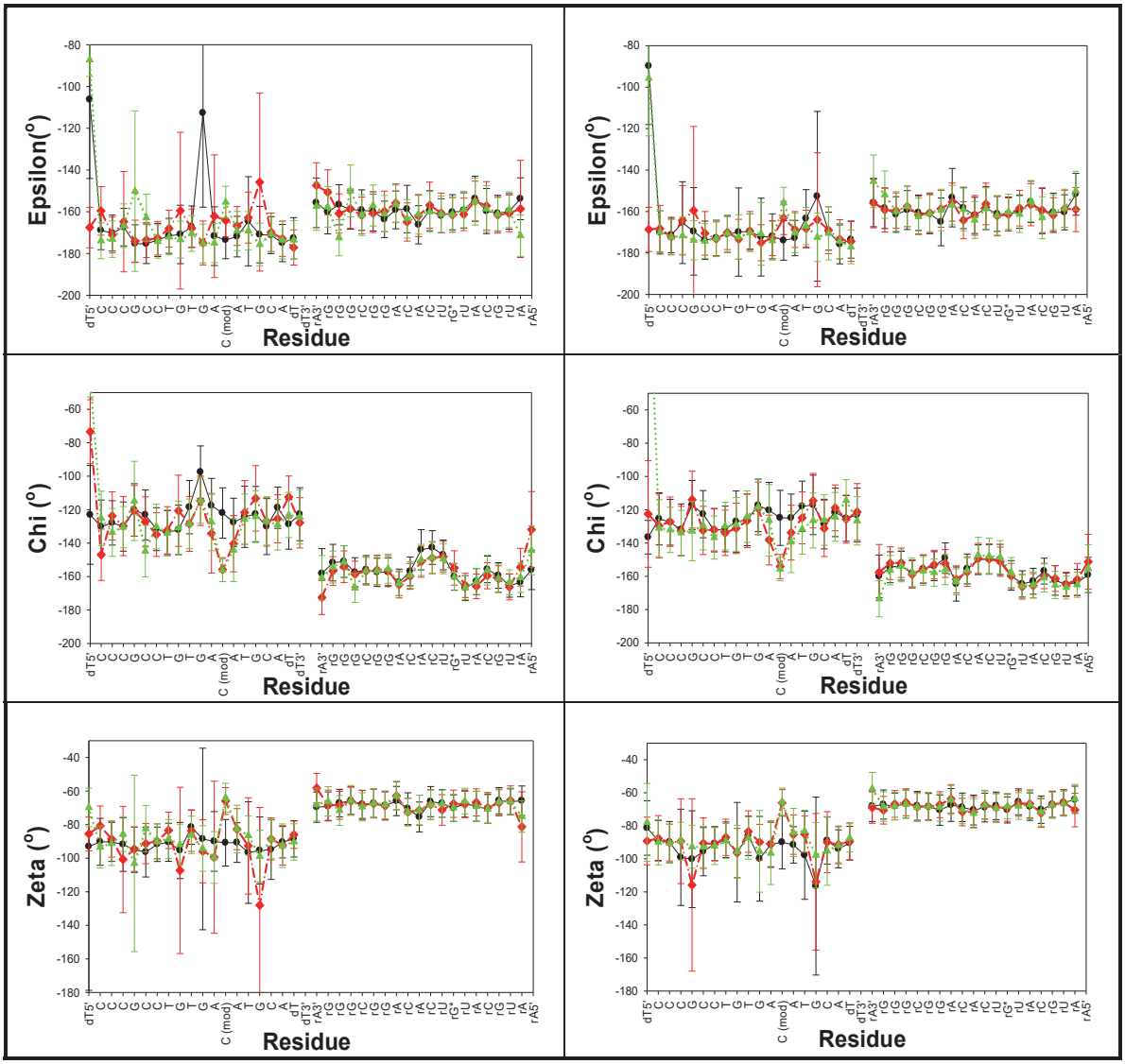
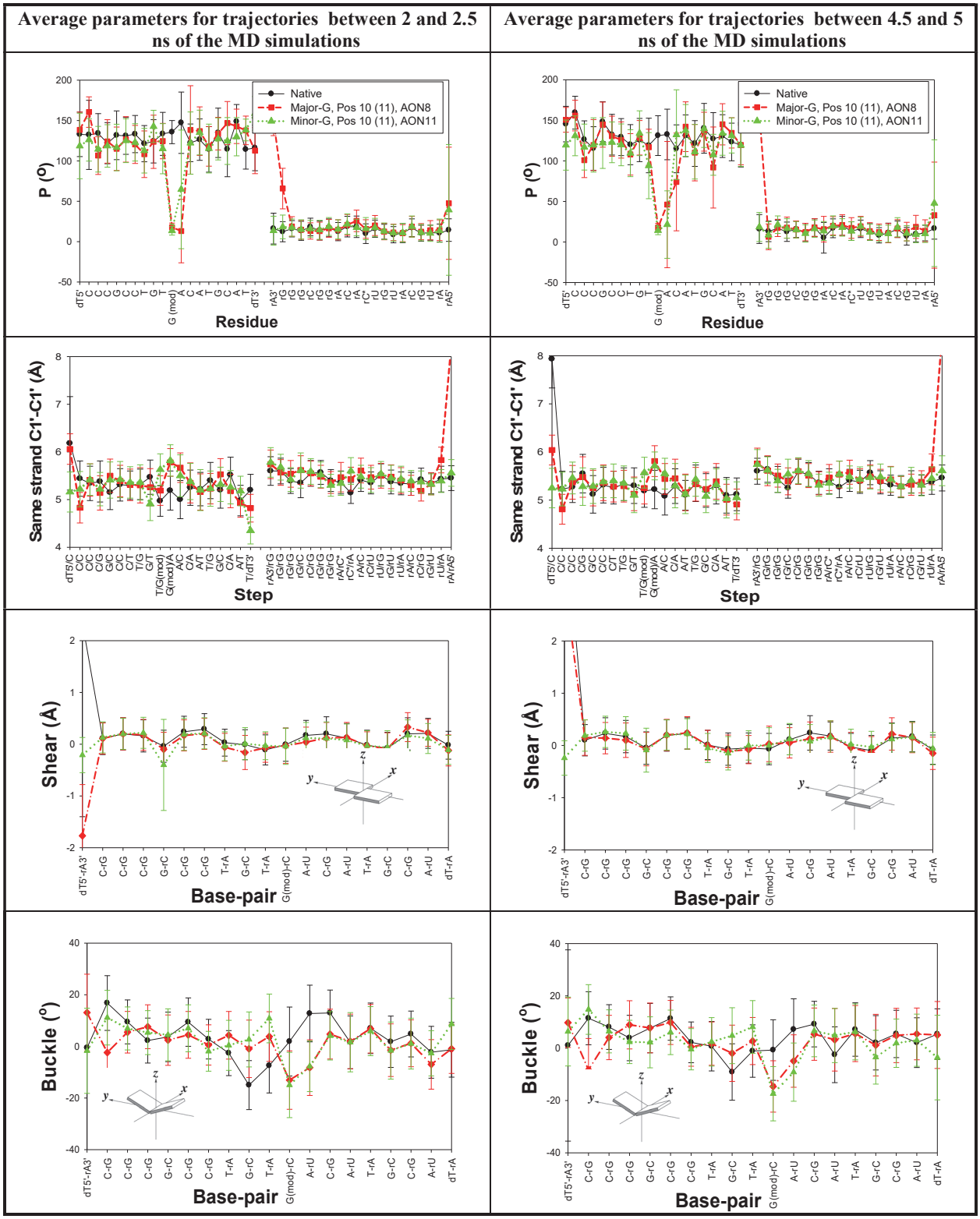
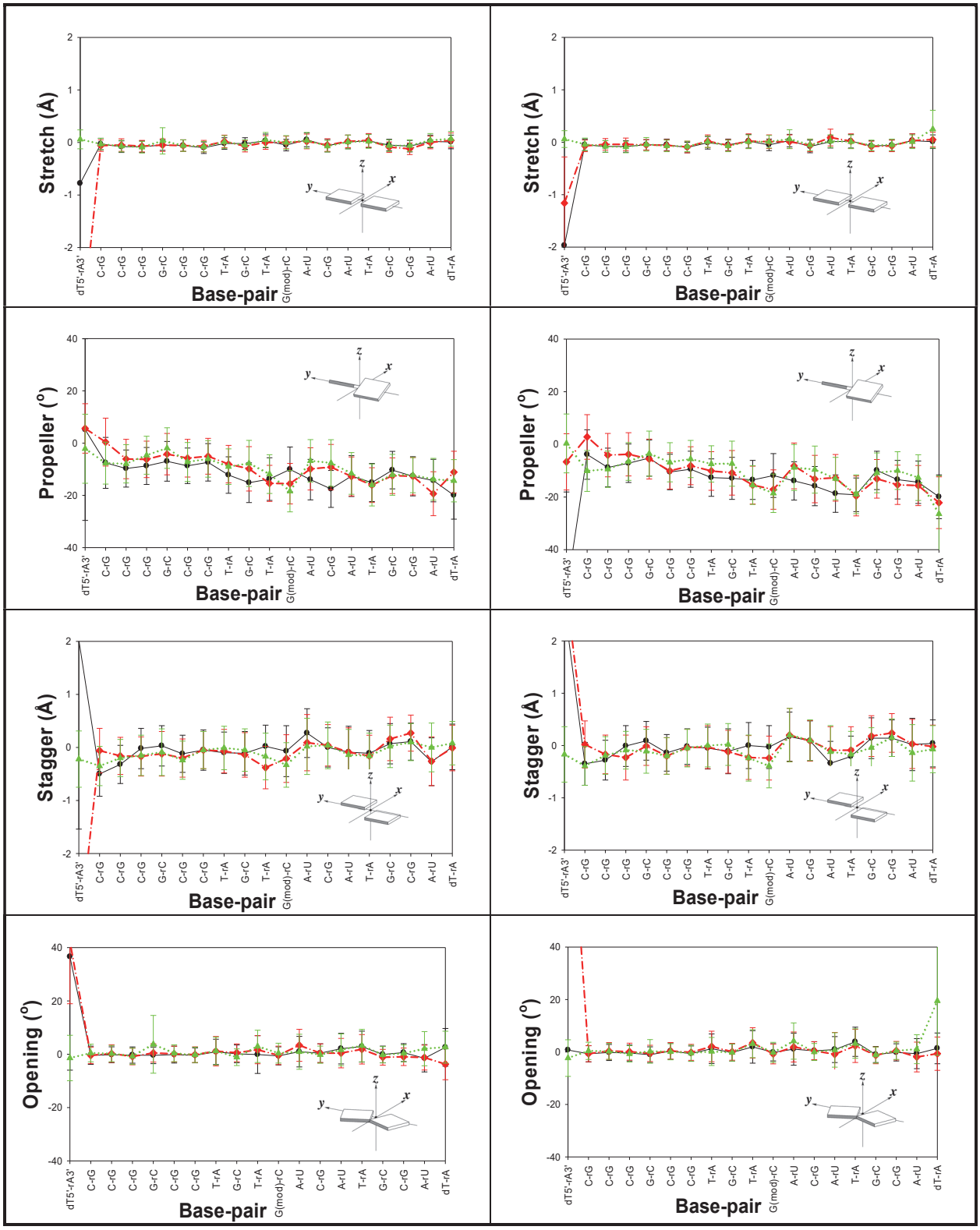
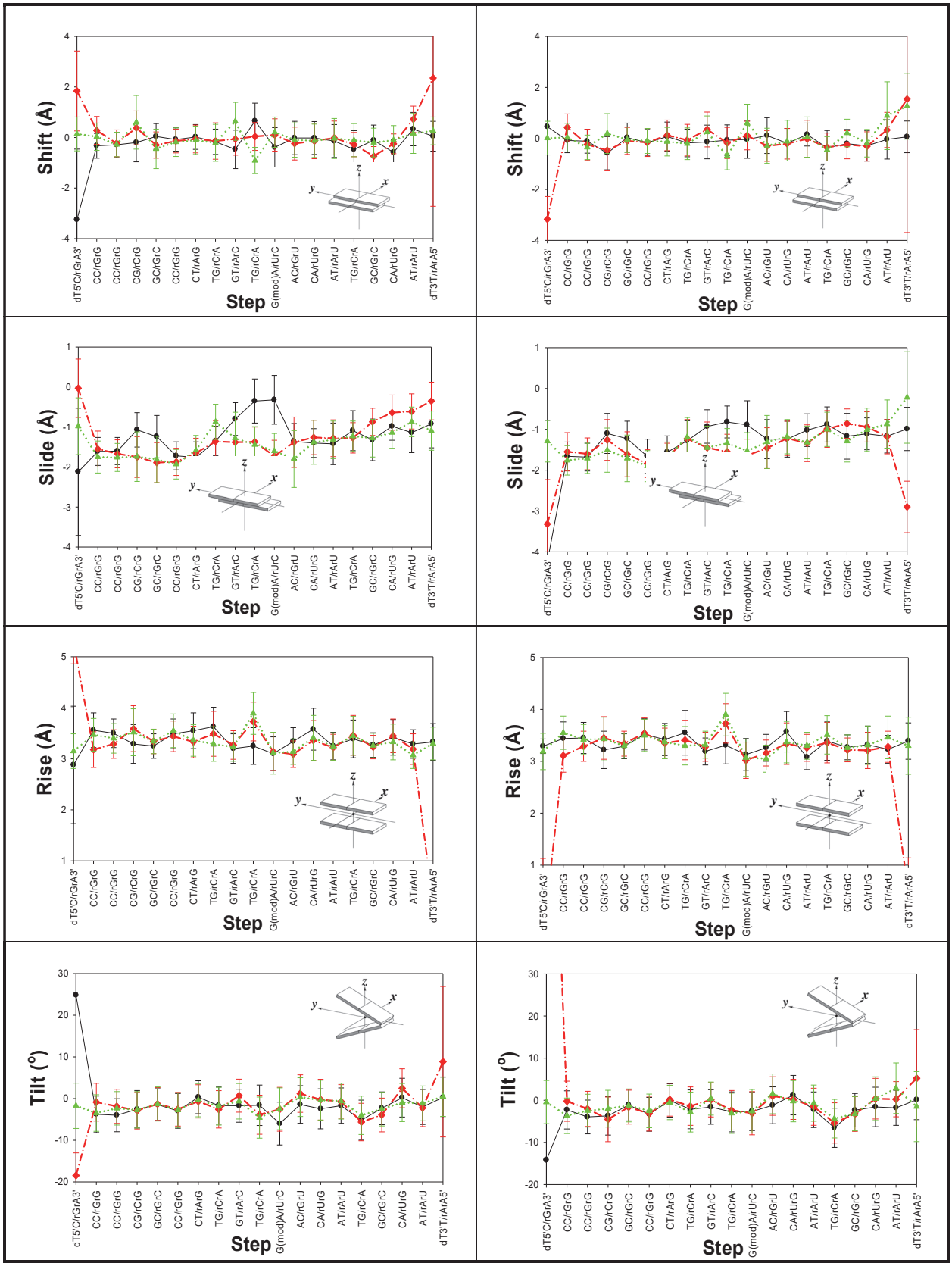

Epsilon(°)
Chi (°)
Zeta (°)
Residue

Figure SIII.7. Geometrical parameters of the native (black circles) and 7′(R/S)-Me-cLNA-G modified AON-RNA duplexes [position 10 modification, AON8 for R- (red squares) and AON11 for S- (green triangles) isomers, respectively]. Average values of the pseudorotational phase angle, same strand C1'-C1' distances, local base-pair, local base-pair step and local base pair helical parameters are shown for two 0.5 ns stretches of the corresponding Amber 12[1] MD trajectories (between 2 and 2.5 ns and 4.5 and 5 ns) using individual snapshots (2500 structures per 0.5 ns) analyzed by 3DNA.[2]




Stretch (Å)
Propeller (°)
Stagger (Å)
Opening (°)
Base-pair
dT5'-rA3'
C-rG
G-rC
T-rA
A-rU
G(mod)-rC
dT-rA
z
x
y


Shift (Å)
Slide (Å)
Rise (Å)
Tilt (°)
Step
dT5'C/rGrA3'
CC/rGrG
CC/rGrG
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GC/rGrC
CC/rGrG
CT/rArG
TG/rCrA
GT/rArC
TG/rCrA
G(mod)A/rUrC
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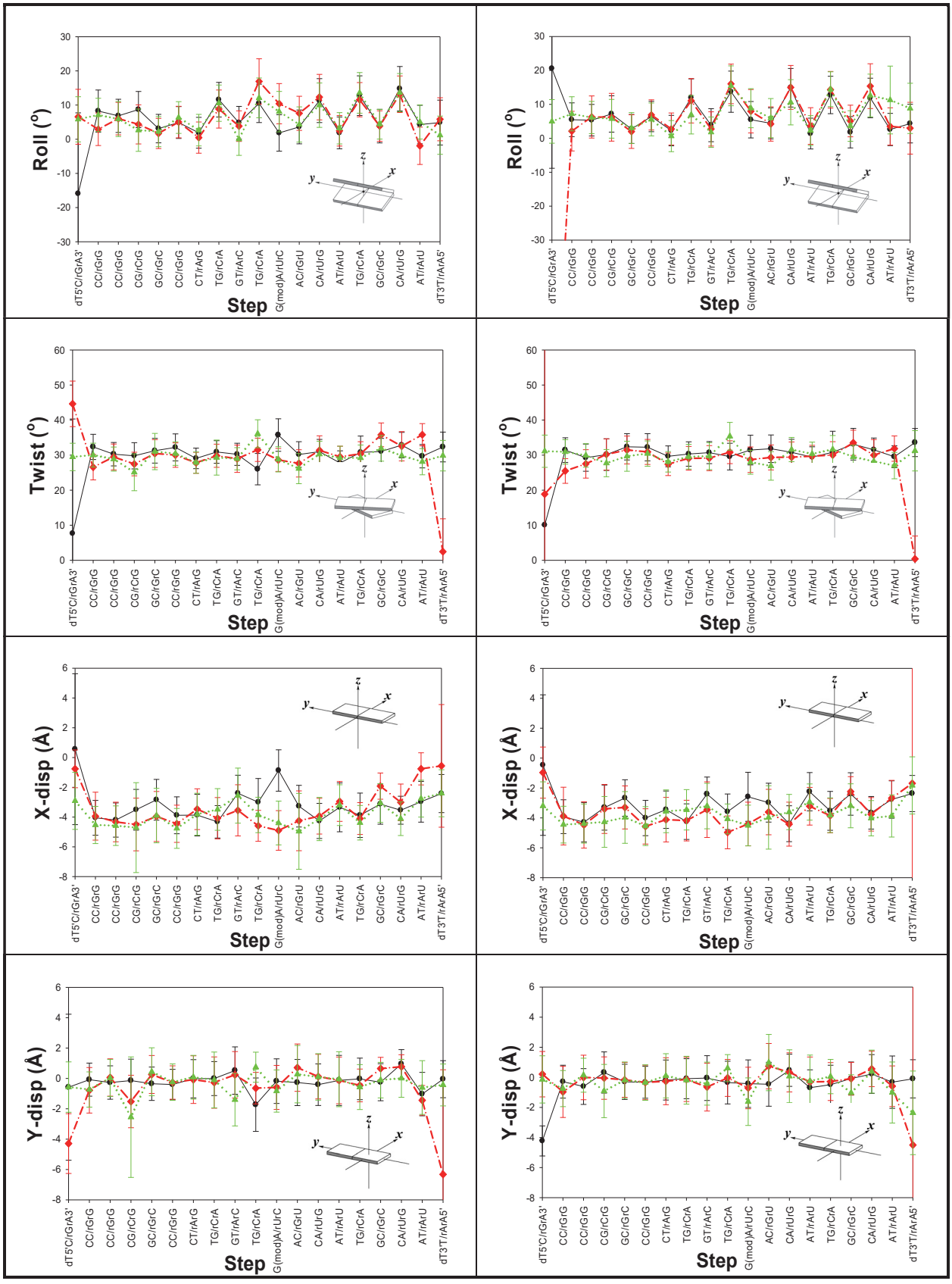
dT3'T/rArA5'


Roll (°)
Twist (°)
X-disp (Å)
Y-disp (Å)
Step
dT5'C/rGrA3'
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CC/rGrG
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GC/rGrC
CC/rGrG
CT/rArG
TG/rCrA
GT/rArC
TG/rCrA
G(mod)A/rUrC
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AT/rArU
dT3'T/rArA5'

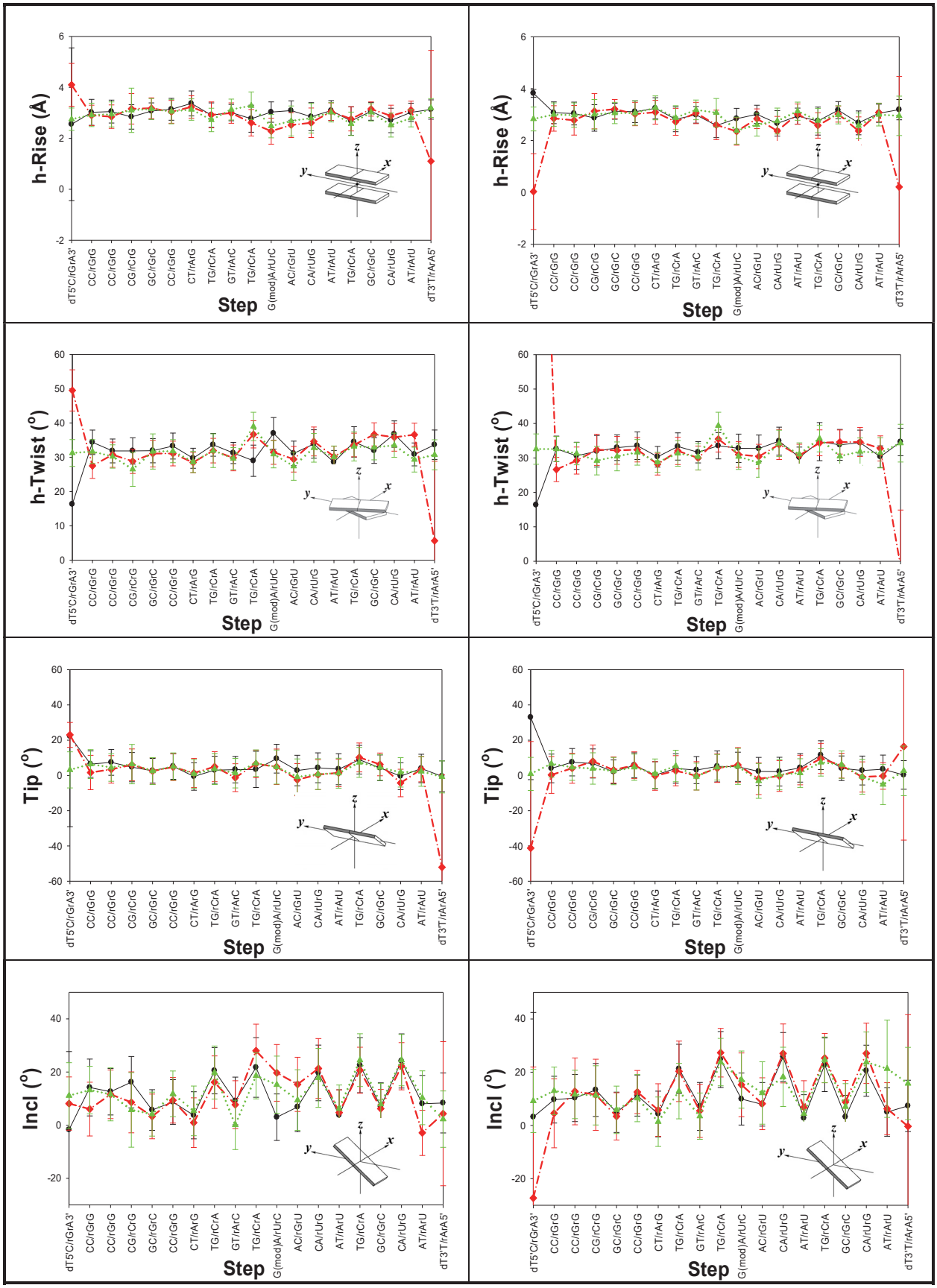
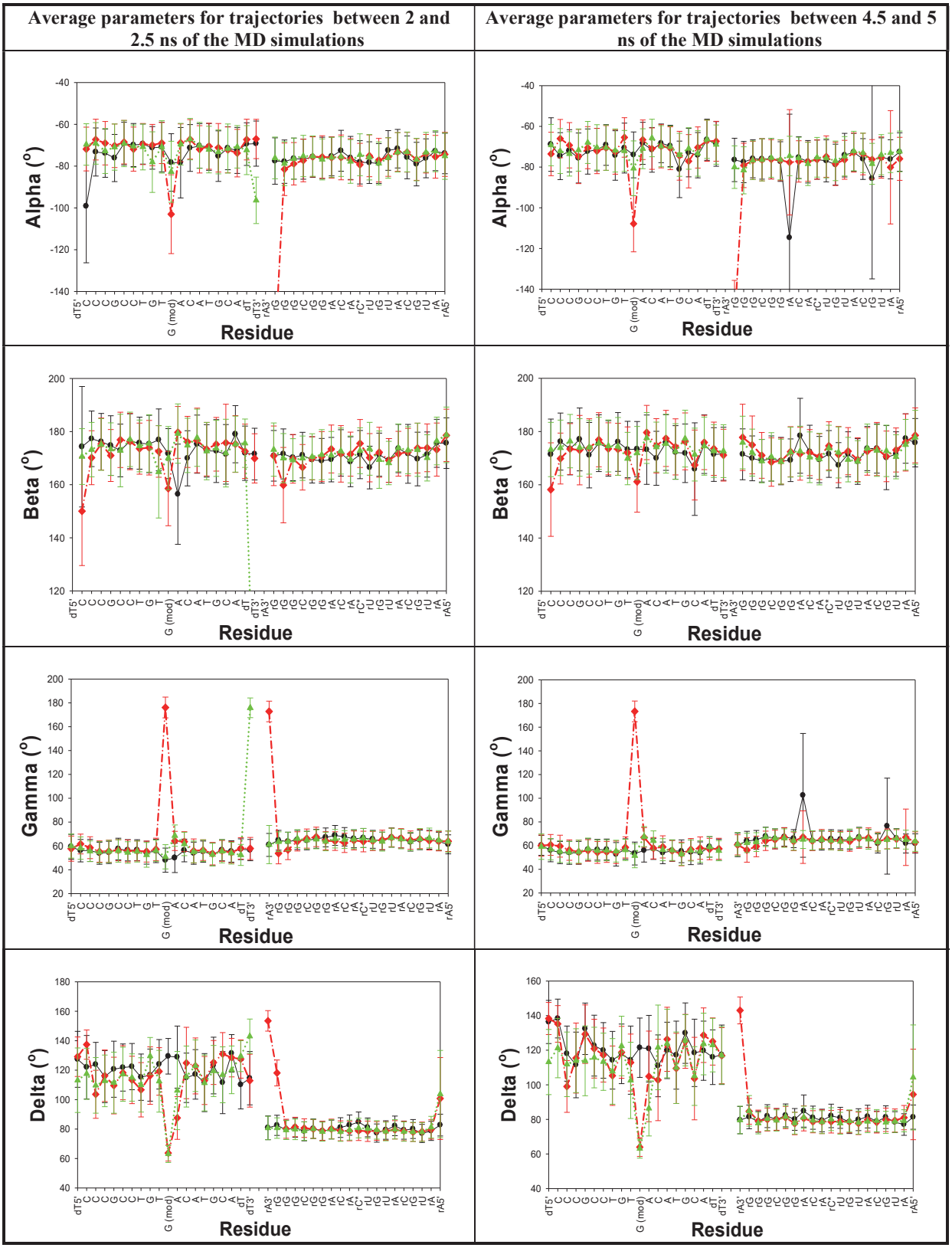

h-Rise (Å)
h-Twist (°)
Tip (°)
Incl (°)
Step
dT5'C/rGrA3'
CC/rGrG
CC/rGrG
CG/rCrG
GC/rGrC
CC/rGrG
CT/rArG
TG/rCrA
GT/rArC
TG/rCrA
G(mod)A/rUrC
AC/rGrU
CA/rUrG
AT/rArU
TG/rCrA
GC/rGrC
CA/rUrG
AT/rArU
dT3'T/rArA5'
z
y
x

Figure SIII.8. Major endocyclic torsions (α, β, γ, δ, ε, ζ, χ)[3] of the native (black circles) and 7′(R/S)-Me-cLNA-G modified AON-RNA duplexes [position 10 modification, AON8 for R- (red squares) and AON11 for S- (green triangles) isomers, respectively] obtained using Amber 12[1] MD trajectories. Average values are shown for two 0.5 ns stretches of the MD trajectories between 2 and 2.5 ns and 4.5 and 5 ns using individual snapshots (2500 structures per 0.5 ns) analyzed by 3DNA.[2]



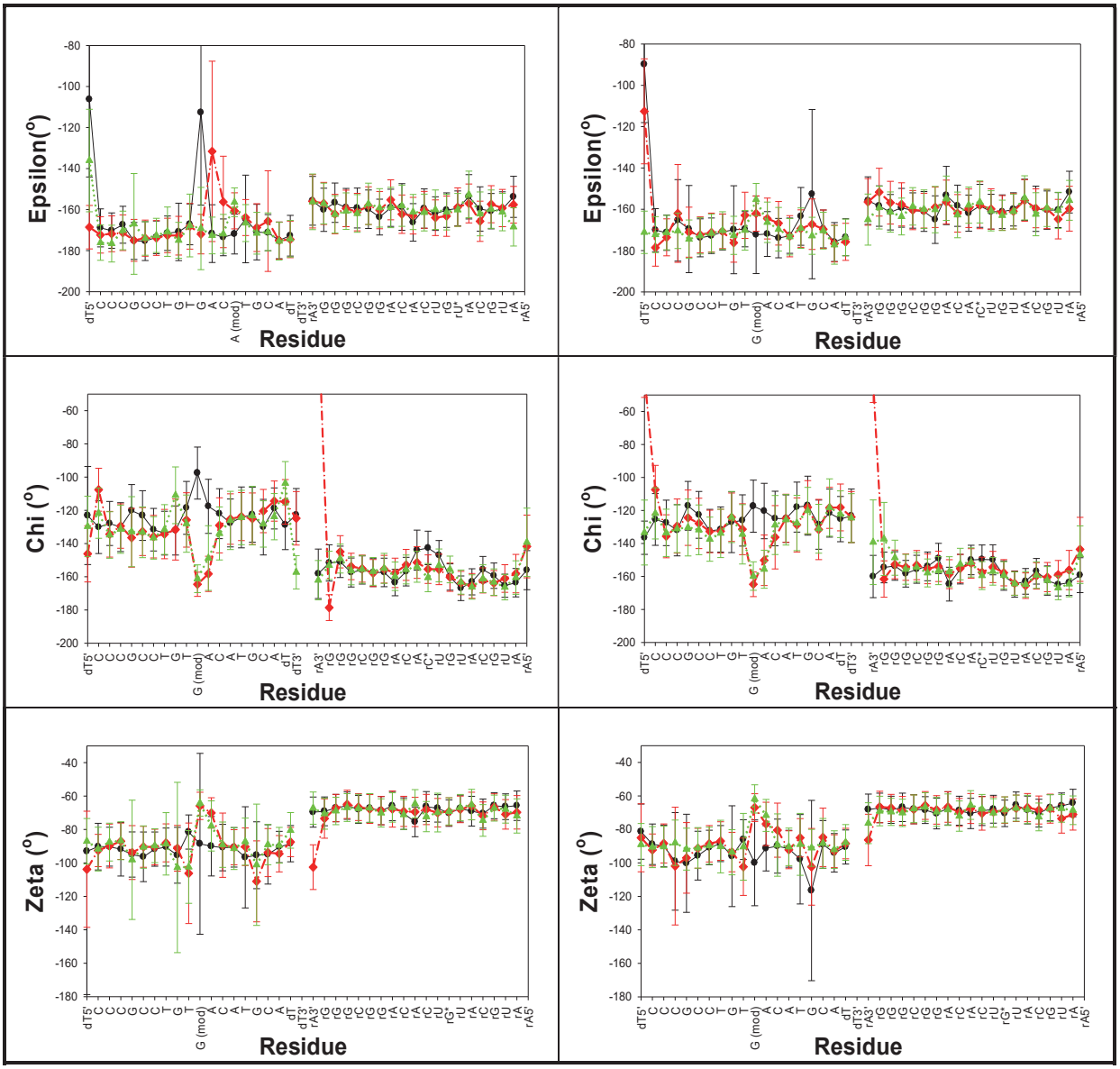
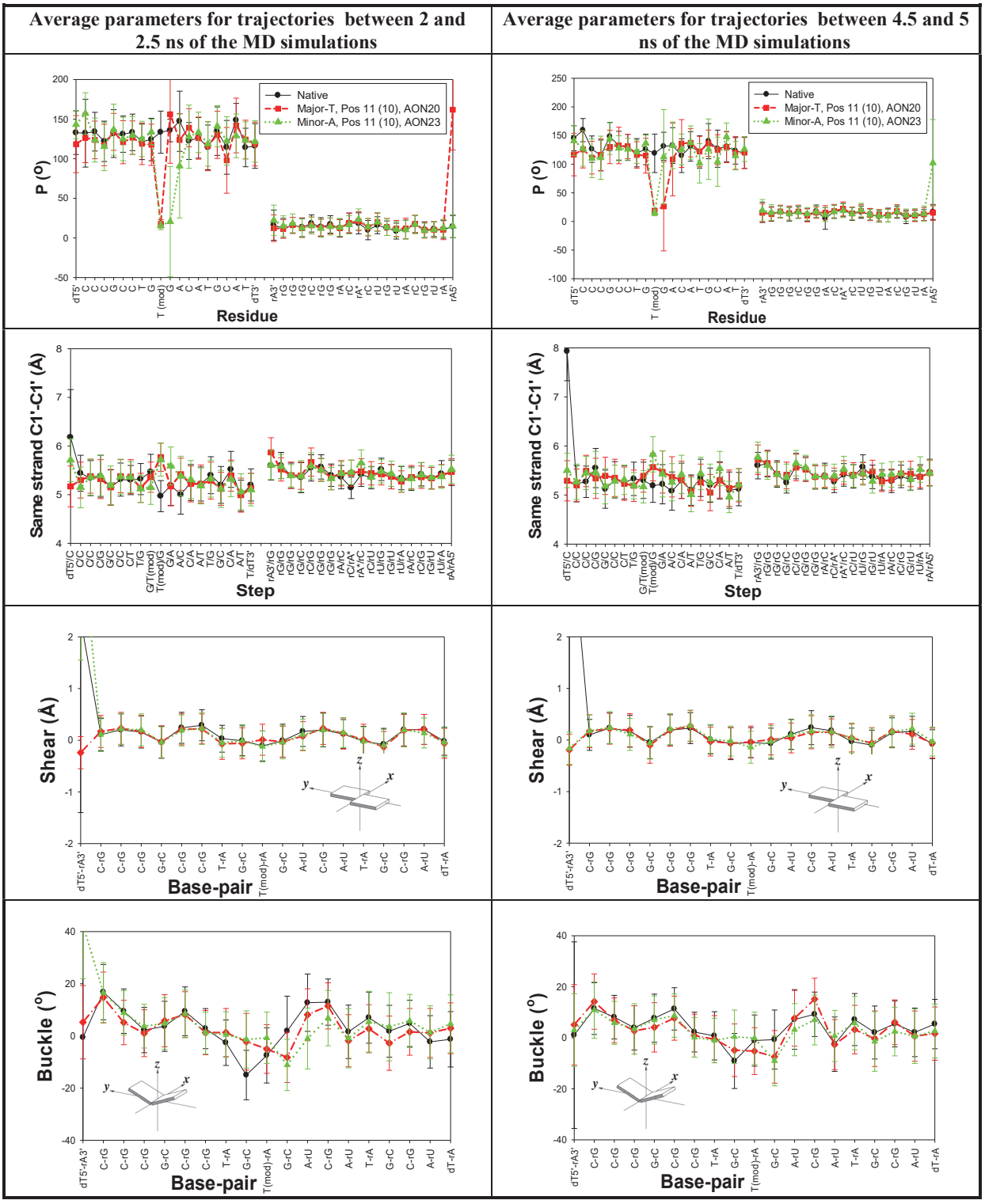
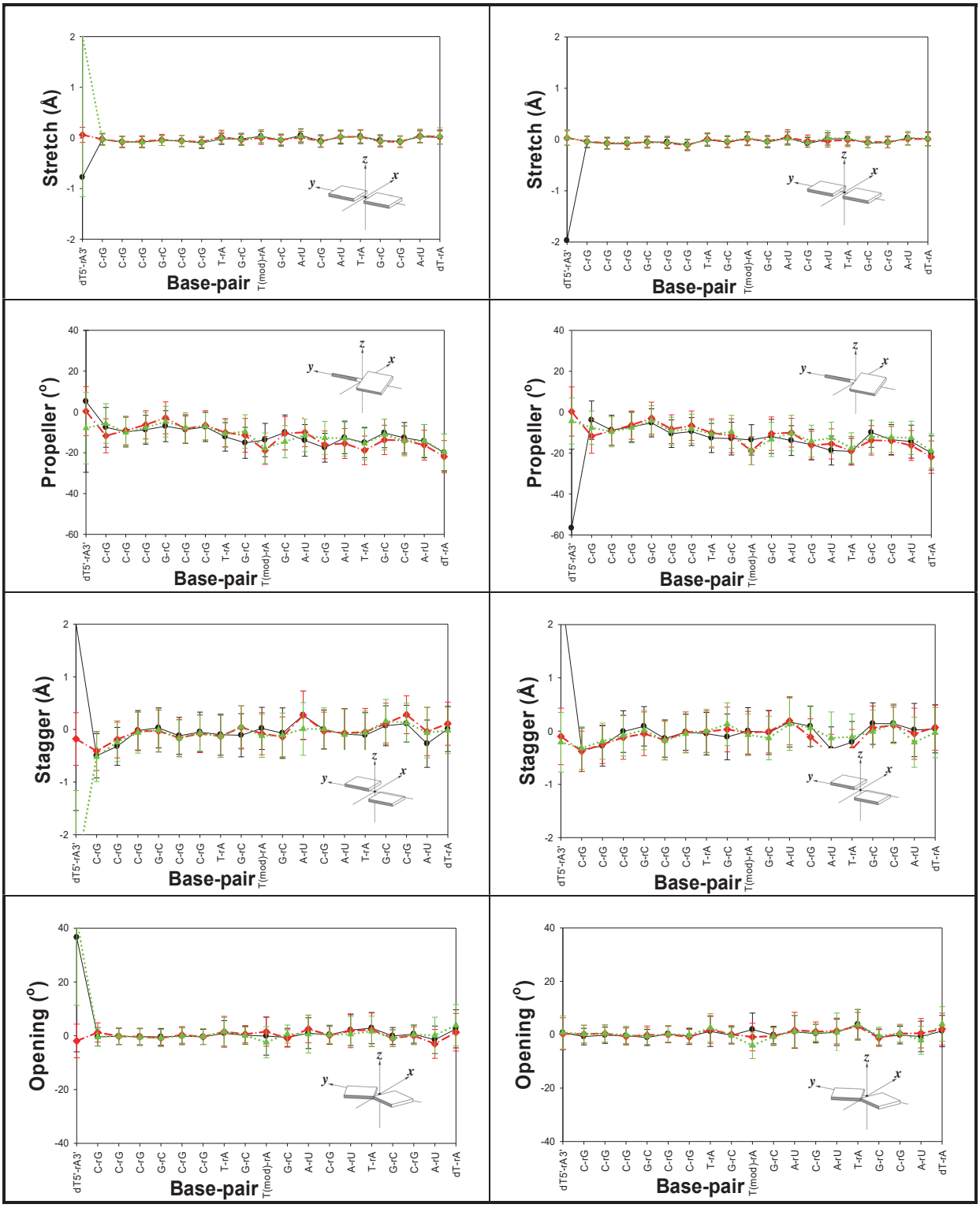
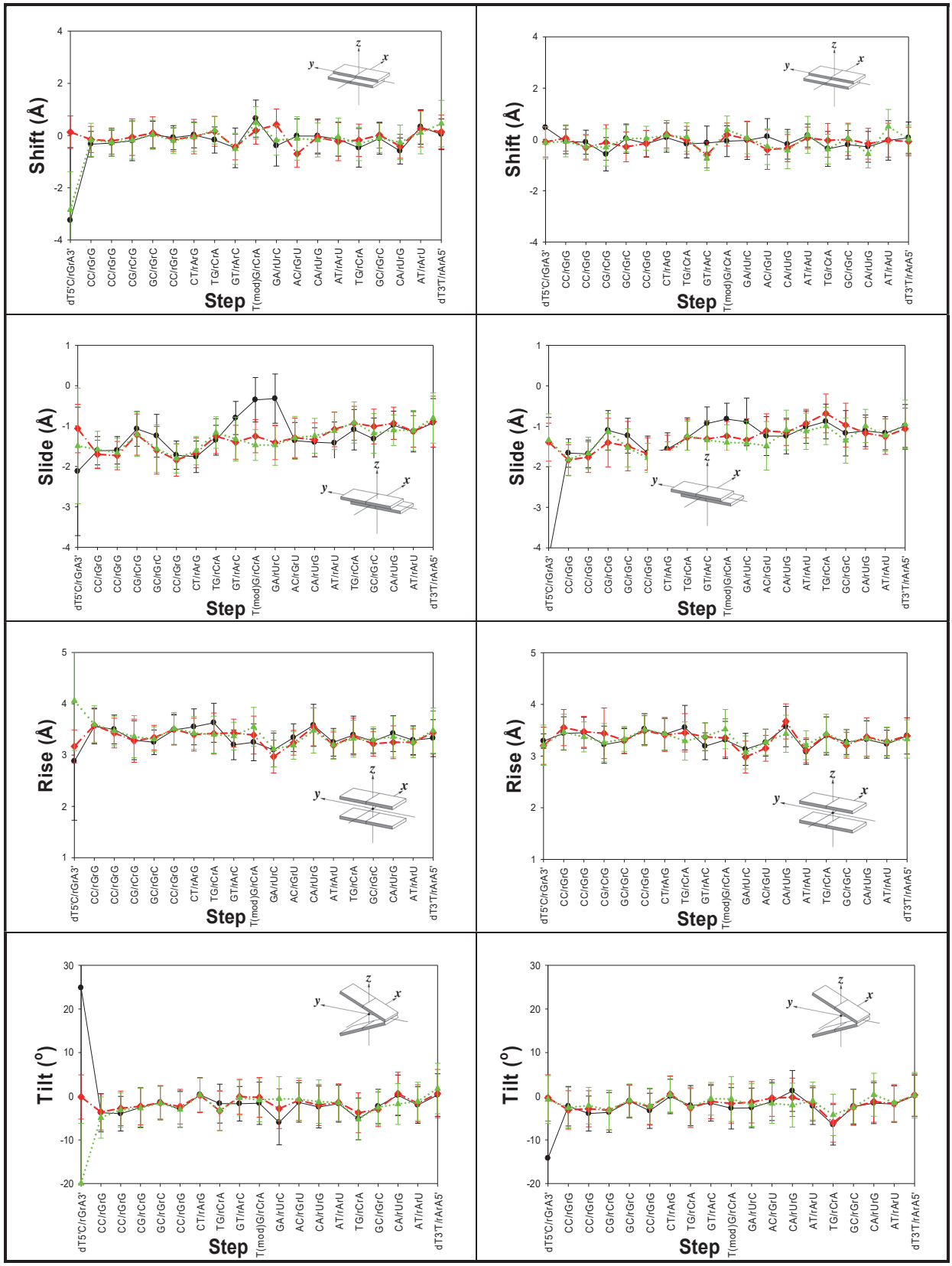
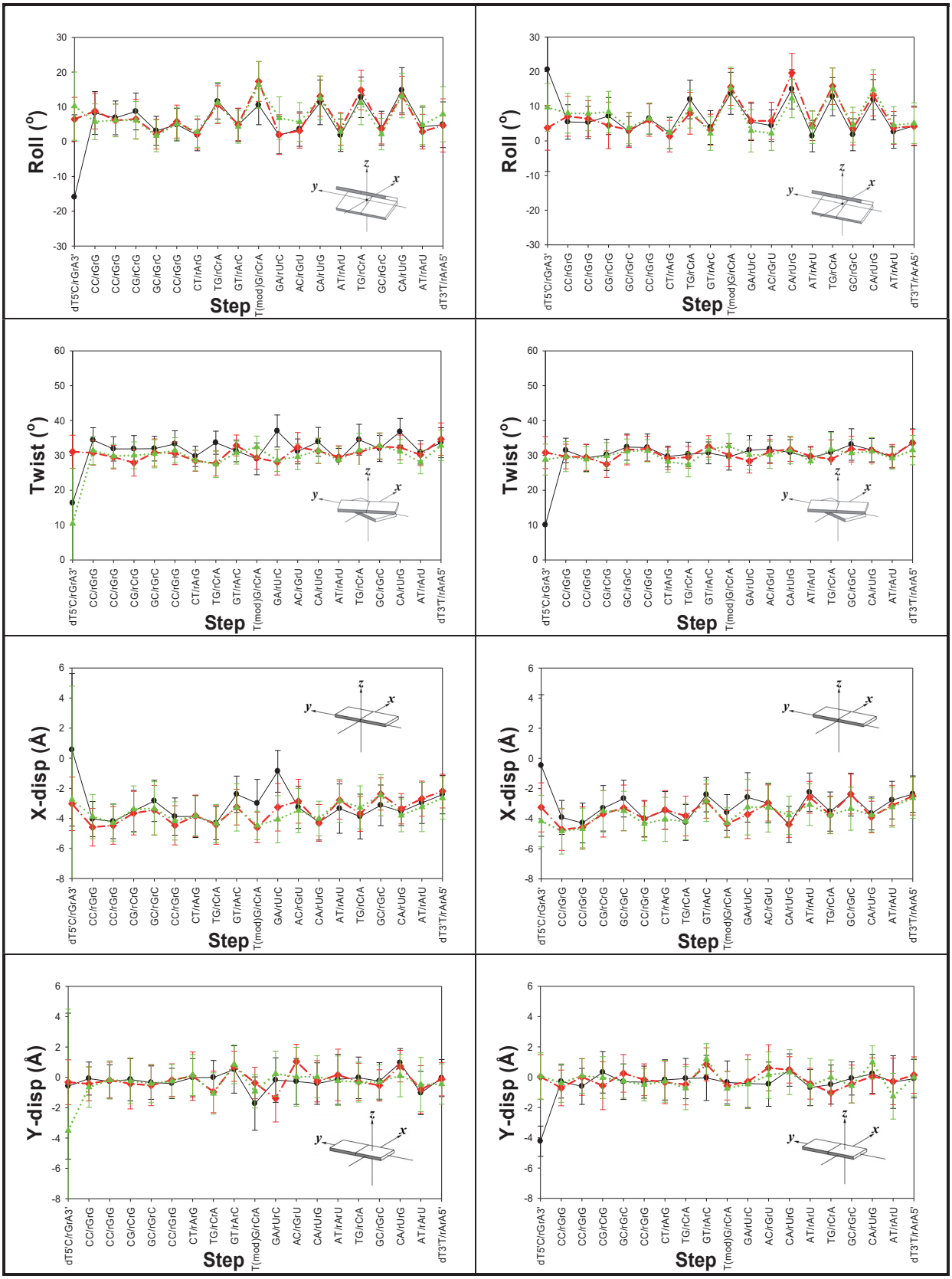

Epsilon(°)
Residue
Chi (°)
Zeta (°)
A (mod)
G (mod)

Figure SIII.9 Geometrical parameters of the native (black circles) and 7′(R/S)-Me-cLNA-T modified AON-RNA duplexes [position 11 modification, AON20 for R- (red squares) and AON23 for S- (green triangles) isomers, respectively]. Average values of the pseudorotational phase angle, same strand C1'-C1' distances, local base-pair, local base-pair step and local base pair helical parameters are shown for two 0.5 ns stretches of the corresponding Amber 12[1] MD trajectories (between 2 and 2.5 ns and 4.5 and 5 ns) using individual snapshots (2500 structures per 0.5 ns) analyzed by 3DNA.[2]




Stretch (Å)
Propeller (°)
Stagger (Å)
Opening (°)
Base-pair
dT5'-rA3'
C-rG
C-rG
C-rG
G-rC
C-rG
C-rG
T-rA
G-rC
T(mod)-rA
G-rC
A-rU
C-rG
A-rU
T-rA
G-rC
C-rG
A-rU
dT-rA
z
x
y


Shift (Å)
Slide (Å)
Rise (Å)
Tilt (°)
Step
dT5'C/rGrA3'
CC/rGrG
CC/rGrG
CG/rCrG
GC/rGrC
CC/rGrG
CT/rArG
TG/rCrA
GT/rArC
T(mod)G/rCrA
GA/rUrC
AC/rGrU
CA/rUrG
AT/rArU
TG/rCrA
GC/rGrC
CA/rUrG
AT/rArU
dT3'T/rArA5'


Roll (°)
Twist (°)
X-disp (Å)
Y-disp (Å)
Step
dT5'C/rGrA3'
CC/rGrG
CC/rGrG
CG/rCrG
GC/rGrC
CC/rGrG
CT/rArG
TG/rCrA
GT/rArC
T(mod)G/rCrA
GA/rUrC
AC/rGrU
CA/rUrG
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TG/rCrA
GC/rGrC
CA/rUrG
AT/rArU
dT3'T/rArA5'

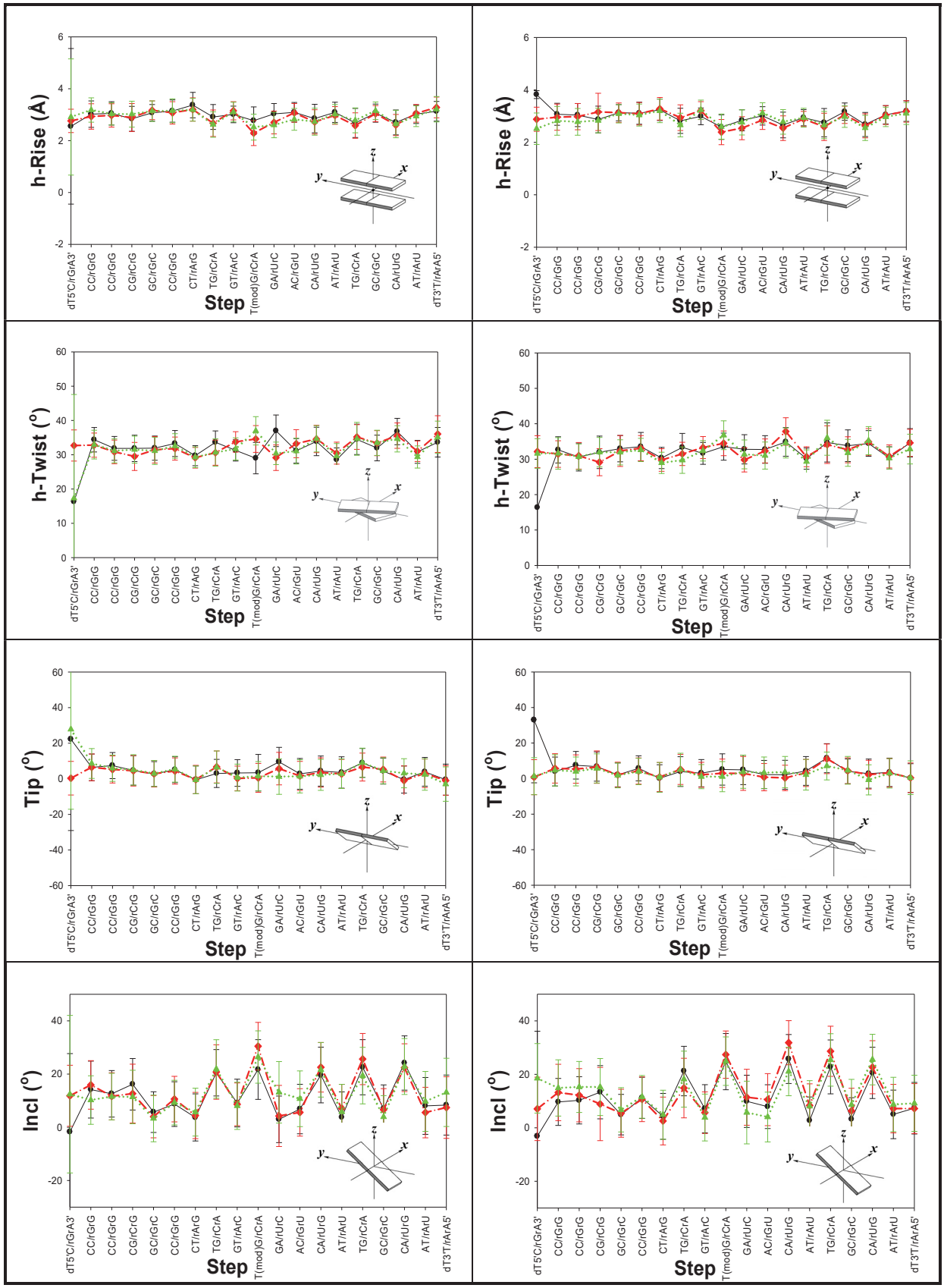
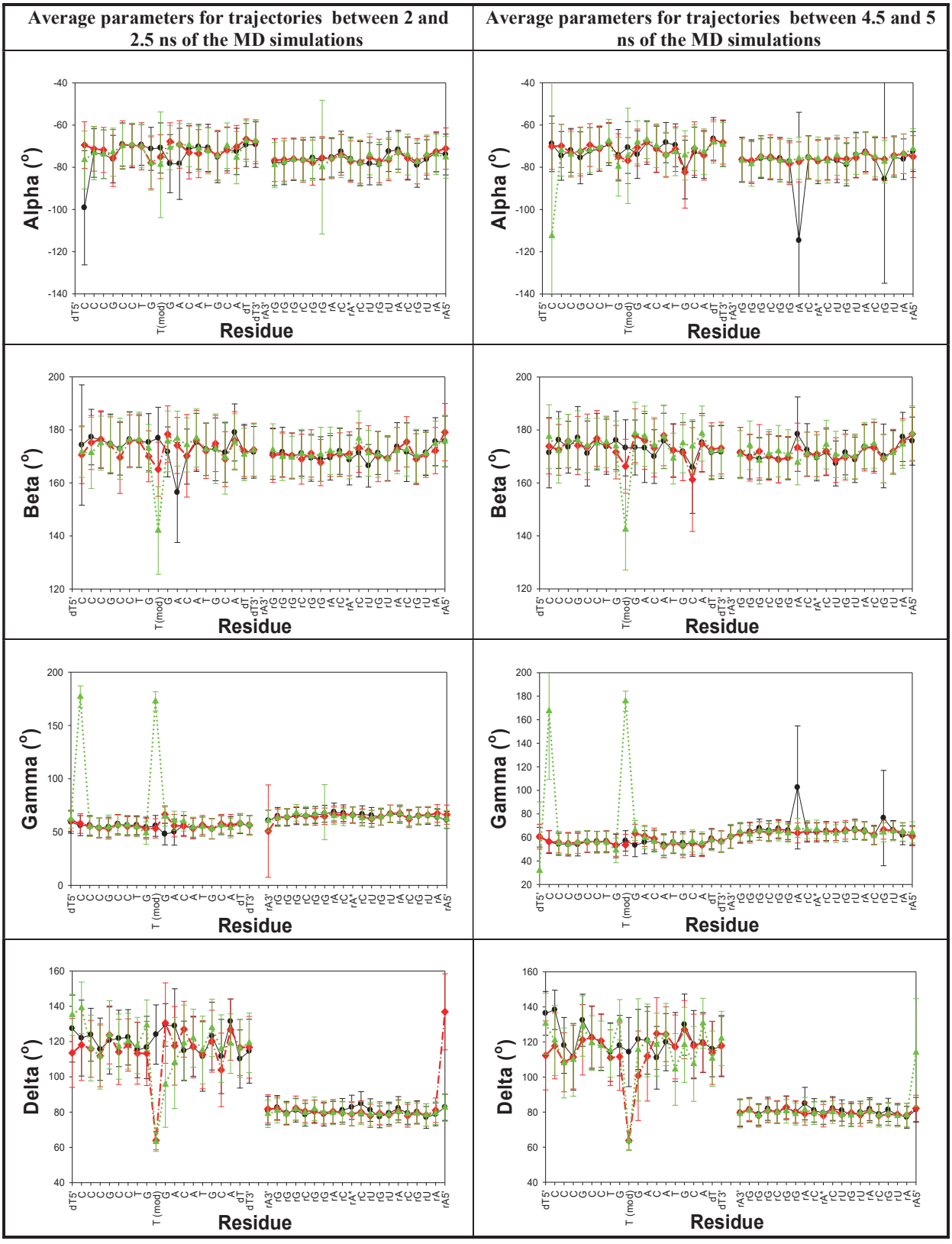

h-Rise (Å)
h-Twist (°)
Tip (°)
Incl (°)
Step
dT5'C/rGrA3'
CC/rGrG
CC/rGrG
CG/rCrG
GC/rGrC
CC/rGrG
CT/rArG
TG/rCrA
GT/rArC
T(mod)G/rCrA
GA/rUrC
AC/rGrU
CA/rUrG
AT/rArU
TG/rCrA
GC/rGrC
CA/rUrG
AT/rArU
dT3'T/rArA5'

Figure SIII.10. Major endocyclic torsions (α, β, γ, δ, ε, ζ, χ)[3] of the native (black circles) and 7′(R/S)-Me-cLNA-T modified AON-RNA duplexes [position 11 modification, AON20 for R- (red squares) and AON23 for S- (green triangles) isomers, respectively] obtained using Amber 12[1] MD trajectories. Average values are shown for two 0.5 ns stretches of the MD trajectories between 2 and 2.5 ns and 4.5 and 5 ns using individual snapshots (2500 structures per 0.5 ns) analyzed by 3DNA.[2]



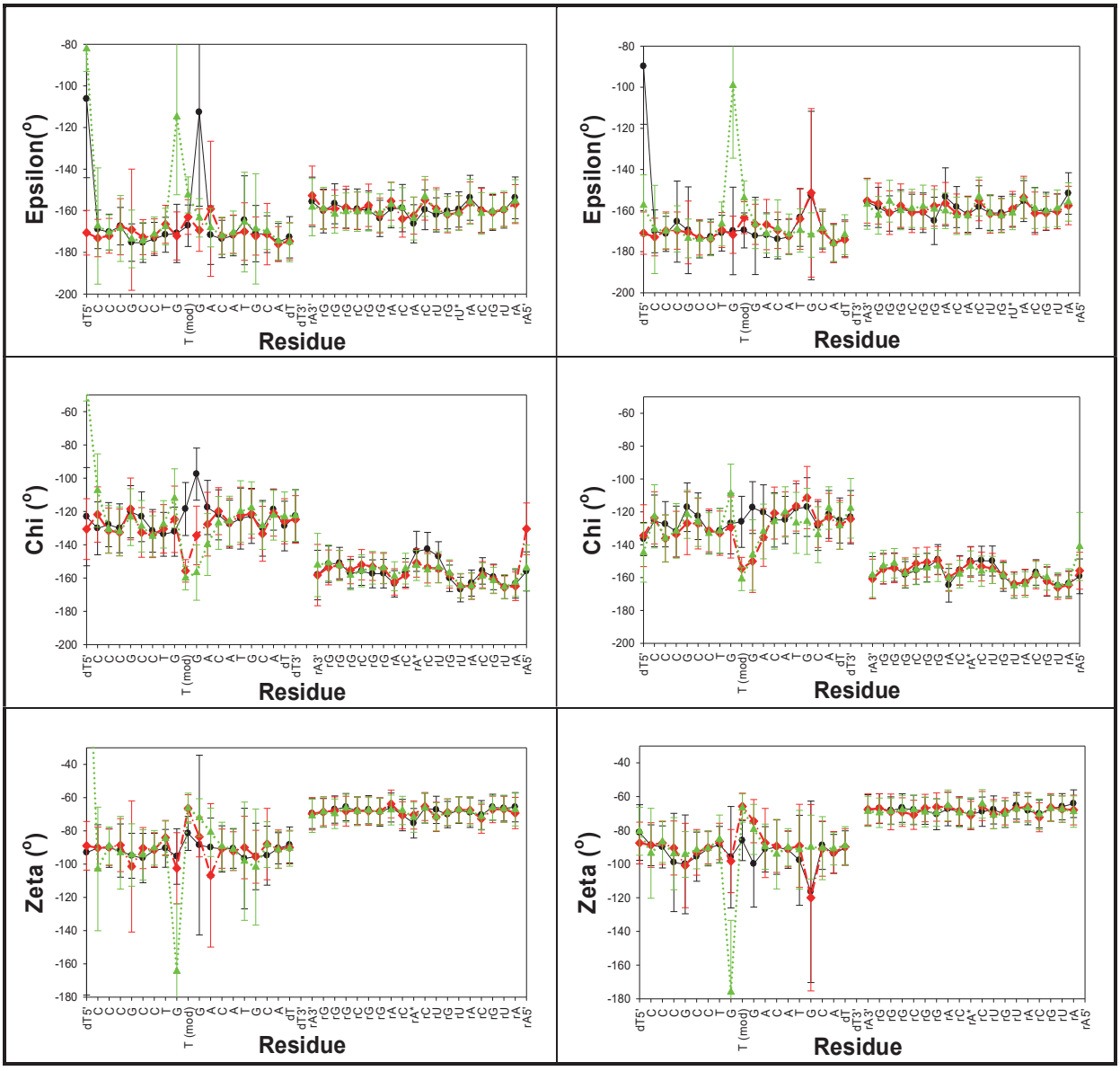

Epsilon(°)
Chi (°)
Zeta (°)
Residue
dT5' C C C C G C C T G T (mod) G A C A T G C A dT dT3' rA3' rG rG rC rG rA rC* rU rG rU rA rC rG rU rA rA5'

Table SIII.19. Atomic charges, atomic names and types for the **native deoxy-A nucleotide** from the standard Amber 94 force field DNA library as implemented in Amber 12[1] with modifications by Pérez *et al.*[4] and for the **modified *7′(R- and S-)*-Me-cLNA-A nucleotides** obtained from the HF/6-31G** *ab initio* geometry optimizations performed using GAUSSIAN 03.[5]

Native deoxy-A nucleotide*						***7′R*-Me-cLNA-A nucleotide**						***7′S*-Me-cLNA-A nucleotide**					
Atom	**Atom Type**	**X**	**Y**	**Z**	**Charge**	**Atom**	**Atom Type**	**X**	**Y**	**Z**	**Charge**	**Atom**	**Atom Type**	**X**	**Y**	**Z**	**Charge**
"P"	"P"	2.314	1.777	-0.478	1.1659	**"P"**	"P"	-9.757	7.048	7.872	1.1659	**"P"**	"P"	-9.710	7.000	8.000	1.1659
"O1P"	"O2"	1.933	3.073	-1.082	-0.7761	**"O1P"**	"O2"	-8.283	6.977	7.763	-0.7350	**"O1P"**	"O2"	-8.230	7.000	8.000	-0.7349
"O2P"	"O2"	3.157	0.872	-1.292	-0.7761	**"O2P"**	"O2"	-10.421	8.363	8.012	-0.7350	**"O2P"**	"O2"	-10.446	8.284	8.000	-0.7349
"O5'"	"OS"	2.994	2.142	0.923	-0.4954	**"O5'"**	"OS"	-10.215	6.119	9.104	-0.6501	**"O5'"**	"OS"	-10.212	6.133	9.260	-0.6498
"C5'"	"CI"	2.156	2.552	2.020	-0.0069	**"C5'"**	"CT"	-9.767	6.397	10.411	0.1303	**"C5'"**	"CT"	-9.875	6.522	10.572	0.1303
"H5'1"	"H1"	1.453	1.754	2.258	0.0754	**"H5'1"**	"H1"	-10.062	7.407	10.697	0.1467	**"H5'1"**	"H1"	-10.239	7.532	10.764	0.1471
"H5'2"	"H1"	1.605	3.450	1.741	0.0754	**"H5'2"**	"H1"	-8.680	6.317	10.438	0.1098	**"H5'2"**	"H1"	-8.791	6.503	10.681	0.1101
"C4'"	"CT"	3.008	2.848	3.243	0.1629	**"C4'"**	"CT"	-10.369	5.393	11.389	0.2320	**"C4'"**	"CT"	-10.498	5.555	11.575	0.2286
"H4'"	"H1"	2.447	3.477	3.934	0.1176	**"C9"**	"CT"	-9.700	5.430	12.763	-0.1983	**"C9"**	"CT"	-9.990	5.769	13.000	-0.1984
"O4'"	"OS"	3.228	1.605	3.977	-0.3691	**"O4'"**	"OS"	-11.761	5.573	11.595	-0.7200	**"O4'"**	"OS"	-11.909	5.675	11.669	-0.7201
"C1'"	"CT"	4.559	1.151	3.778	0.0431	**"C1'"**	"CT"	-12.242	4.330	12.078	0.5071	**"C1'"**	"CT"	-12.362	4.443	12.205	0.5108
"H1'"	"H2"	5.072	1.095	4.737	0.1838	**"H1'"**	"H2"	-12.767	4.452	13.025	0.1714	**"H1'"**	"H2"	-12.961	4.601	13.102	0.1706
"N9"	"N*"	4.539	-0.297	3.316	-0.0268	**"N9"**	"N*"	-13.120	3.692	11.080	-0.8064	**"N9"**	"N*"	-13.133	3.693	11.196	-0.8090
"C8"	"CK"	4.337	-0.846	2.077	0.1607	**"C8"**	"CK"	-12.809	3.231	9.826	0.3760	**"C8"**	"CK"	-12.709	3.166	10.003	0.3757
"H8"	"H5"	4.152	-0.207	1.226	0.1877	**"H8"**	"H5"	-11.833	3.352	9.380	0.1860	**"H8"**	"H5"	-11.710	3.308	9.618	0.1865
"N7"	"NB"	4.453	-2.141	2.049	-0.6175	**"N7"**	"NB"	-13.803	2.648	9.215	-0.5927	**"N7"**	"NB"	-13.626	2.491	9.367	-0.5922
"C5"	"CB"	4.754	-2.480	3.363	0.0725	**"C5"**	"CB"	-14.841	2.704	10.140	0.0677	**"C5"**	"CB"	-14.730	2.553	10.211	0.0675
"C6"	"CA"	4.998	-3.708	3.989	0.6897	**"C6"**	"CA"	-16.165	2.238	10.115	0.6428	**"C6"**	"CA"	-16.025	2.016	10.127	0.6427
"N6"	"N2"	4.977	-4.883	3.346	-0.9123	**"N6"**	"N2"	-16.704	1.604	9.064	-0.7663	**"N6"**	"N2"	-16.453	1.286	9.088	-0.7661
"H61"	"H"	5.161	-5.739	3.851	0.4167	**"H61"**	"H"	-17.661	1.287	9.102	0.3226	**"H61"**	"H"	-17.395	0.921	9.083	0.3226
"H62"	"H"	4.777	-4.914	2.356	0.4167	**"H62"**	"H"	-16.152	1.445	8.233	0.3314	**"H62"**	"H"	-15.835	1.100	8.312	0.3314
"N1"	"NC"	5.265	-3.689	5.302	-0.7624	**"N1"**	"NC"	-16.913	2.439	11.209	-0.6675	**"N1"**	"NC"	-16.860	2.251	11.149	-0.6672
"C2"	"CQ"	5.285	-2.520	5.935	0.5716	**"C2"**	"CQ"	-16.382	3.062	12.251	0.3434	**"C2"**	"CQ"	-16.438	2.970	12.179	0.3434
"H2"	"H5"	5.498	-2.482	6.993	0.0598	**"H2"**	"H5"	-17.037	3.187	13.100	0.1549	**"H2"**	"H5"	-17.159	3.118	12.969	0.1552
"N3"	"NC"	5.073	-1.309	5.456	-0.7417	**"N3"**	"NC"	-15.160	3.550	12.401	-0.6525	**"N3"**	"NC"	-15.256	3.532	12.378	-0.6522
"C4"	"CB"	4.806	-1.356	4.133	0.38	**"C4"**	"CB"	-14.430	3.333	11.284	0.6809	**"C4"**	"CB"	-14.435	3.279	11.333	0.6809
"C3'"	"CT"	4.416	3.378	2.961	0.0713	**"C3'"**	"CT"	-10.204	3.925	11.029	0.2197	**"C3'"**	"CT"	-10.236	4.077	11.333	0.2309

"H3'"	"H1"	4.412	3.941	2.028	0.0985	**"H3'"**	"H1"	-10.712	3.660	10.102	0.1425	**"H3'"**	"H1"	-10.661	3.724	10.394	0.1406
"C2'"	"CT"	5.230	2.096	2.779	-0.0854	**"C2'"**	"CT"	-10.980	3.503	12.262	-0.2180	**"C2'"**	"CT"	-11.079	3.699	12.536	-0.2219
"H2'1"	"HC"	5.668	2.081	1.781	0.0718	**"H2'1"**	"HC"	-11.150	2.431	12.371	0.1581	**"H2'1"**	"HC"	-11.205	2.630	12.708	0.1599
"H2'2"	"HC"	6.025	2.061	3.525	0.0718	**"C31"**	"CT"	-10.228	4.154	13.418	-0.1390	**"C31"**	"CT"	-10.371	4.447	13.660	-0.1373
"O3'"	"OS"	5.030	4.129	3.998	-0.5232	**"O3'"**	"OS"	-8.861	3.497	11.073	-0.6634	**"O3'"**	"OS"	-8.880	3.726	11.501	-0.6628
						"C33"	"CT"	-11.192	4.479	14.555	-0.3242	**"H38"**	"HC"	-8.908	5.902	13.008	0.1429
						"H34"	"HC"	-11.996	5.111	14.176	0.1115	**"H39"**	"HC"	-10.501	6.609	13.470	0.1339
						"H35"	"HC"	-11.614	3.556	14.952	0.1258	**"C33"**	"CT"	-9.139	3.709	14.093	-0.3230
						"H36"	"HC"	-10.659	5.007	15.346	0.1192	**"H34"**	"HC"	-8.658	4.243	14.788	0.1335
						"H37"	"HC"	-9.406	3.525	13.759	0.1485	**"H35"**	"HC"	-8.540	3.571	13.304	0.1124
						"H38"	"HC"	-8.618	5.369	12.651	0.1412	**"H36"**	"HC"	-9.399	2.822	14.474	0.1138
						"H39"	"HC"	-9.993	6.317	13.323	0.1325	**"H37"**	"HC"	-10.988	4.596	14.433	0.1326

Table SIII.20. Atomic charges, atomic names and types for the **native deoxy-G nucleotide** from the standard Amber 94 force field DNA library as implemented in Amber 12[1] with modifications by Pérez *et al.*[4] and for the **modified *7′(R- and S-)*-Me-cLNA-G nucleotides** obtained from the HF/6-31G** *ab initio* geometry optimizations performed using GAUSSIAN 03.[5]

Native deoxy-G nucleotide*						***7′R*-Me-cLNA-G nucleotide**						***7′S*-Me-cLNA-G nucleotide**					
Atom	**Atom Type**	**X**	**Y**	**Z**	**Charge**	**Atom**	**Atom Type**	**X**	**Y**	**Z**	**Charge**	**Atom**	**Atom Type**	**X**	**Y**	**Z**	**Charge**
"P"	"P"	2.314	1.777	-0.478	1.1659	**"P"**	"P"	-9.811	7.004	7.854	1.1659	**"P"**	"P"	-9.710	7.000	8.000	1.1659
"O1P"	"O2"	1.933	3.073	-1.082	-0.7761	**"O1P"**	"O2"	-8.388	6.712	7.567	-0.7364	**"O1P"**	"O2"	-8.230	7.000	8.000	-0.7364
"O2P"	"O2"	3.157	0.872	-1.292	-0.7761	**"O2P"**	"O2"	-10.247	8.401	8.072	-0.7364	**"O2P"**	"O2"	-10.388	8.316	8.000	-0.7364
"O5'"	"OS"	2.994	2.142	0.923	-0.4954	**"O5'"**	"OS"	-10.254	6.134	9.135	-0.6441	**"O5'"**	"OS"	-10.136	6.097	9.250	-0.6441
"C5'"	"CI"	2.156	2.552	2.020	-0.0069	**"C5'"**	"CT"	-9.623	6.322	10.381	0.1439	**"C5'"**	"CT"	-10.008	6.639	10.578	0.1439
"H5'1"	"H1"	1.453	1.754	2.258	0.0754	**"H5'1"**	"H1"	-9.724	7.361	10.695	0.1399	**"H5'1"**	"H1"	-10.623	7.535	10.667	0.1399
"H5'2"	"H1"	1.605	3.450	1.741	0.0754	**"H5'2"**	"H1"	-8.566	6.073	10.287	0.1086	**"H5'2"**	"H1"	-8.966	6.895	10.769	0.1086
"C4'"	"CT"	3.008	2.848	3.243	0.1629	**"C4'"**	"CT"	-10.267	5.406	11.419	0.2260	**"C4'"**	"CT"	-10.652	5.430	11.188	0.2260
"H4'"	"H1"	2.447	3.477	3.934	0.1176	**"C9"**	"CT"	-9.512	5.354	12.747	-0.2175	**"C9"**	"CT"	-10.100	4.659	11.701	-0.2175
"O4'"	"OS"	3.228	1.605	3.977	-0.3691	**"O4'"**	"OS"	-11.599	5.772	11.733	-0.6930	**"O4'"**	"OS"	-11.896	5.703	11.777	-0.6930
"C1'"	"CT"	4.559	1.151	3.778	0.0358	**"C1'"**	"CT"	-12.199	4.601	12.259	0.5132	**"C1'"**	"CT"	-12.695	4.669	11.272	0.5132
"H1'"	"H2"	5.072	1.095	4.737	0.1746	**"H1'"**	"H2"	-12.632	4.783	13.243	0.1615	**"H1'"**	"H2"	-13.296	4.258	12.083	0.1615
"N9"	"N*"	4.500	-0.268	3.327	0.0577	**"N9"**	"N*"	-13.224	4.111	11.319	-0.8022	**"N9"**	"N*"	-13.615	5.215	10.237	-0.8022
"C8"	"CK"	4.268	-0.773	2.063	0.0736	**"C8"**	"CK"	-13.064	3.687	10.025	0.3404	**"C8"**	"CK"	-13.482	5.728	8.962	0.3404
"H8"	"H5"	4.096	-0.100	1.236	0.1997	**"H8"**	"H5"	-12.114	3.713	9.511	0.2128	**"H8"**	"H5"	-12.512	5.756	8.490	0.2128
"N7"	"NB"	4.279	-2.081	2.002	-0.5725	**"N7"**	"NB"	-14.163	3.265	9.467	-0.5397	**"N7"**	"NB"	-14.607	6.148	8.438	-0.5397
"C5"	"CB"	4.535	-2.475	3.310	0.1991	**"C5"**	"CB"	-15.119	3.397	10.469	-0.0238	**"C5"**	"CB"	-15.550	5.900	9.427	-0.0238
"C6"	"C"	4.665	-3.772	3.873	0.4918	**"C6"**	"C"	-16.502	3.075	10.449	0.8188	**"C6"**	"C"	-16.950	6.140	9.446	0.8188
"O6"	"O"	4.578	-4.865	3.316	-0.5699	**"O6"**	"O"	-17.165	2.616	9.522	-0.5932	**"O6"**	"O"	-17.659	6.634	8.570	-0.5932
"N1"	"NA"	4.926	-3.709	5.247	-0.5053	**"N1"**	"NA"	-17.099	3.331	11.675	-0.8346	**"N1"**	"NA"	-17.522	5.732	10.657	-0.8346
"H1"	"H"	5.033	-4.576	5.734	0.3520	**"H1"**	"H"	-18.084	3.123	11.755	0.3304	**"H1"**	"H"	-18.507	5.863	10.767	0.3304
"C2"	"CA"	5.048	-2.547	5.982	0.7432	**"C2"**	"CA"	-16.451	3.834	12.784	0.9173	**"C2"**	"CA"	-16.835	5.165	11.711	0.9173
"N2"	"N2"	5.299	-2.702	7.289	-0.9230	**"N2"**	"N2"	-17.191	3.997	13.889	-0.7611	**"N2"**	"N2"	-17.568	4.844	12.785	-0.7611
"H21"	"H"	5.397	-3.574	7.790	0.4235	**"H21"**	"H"	-18.171	3.754	13.881	0.3071	**"H21"**	"H"	-18.561	4.983	12.907	0.3071
"H22"	"H"	5.381	-1.857	7.836	0.4235	**"H22"**	"H"	-16.766	4.354	14.733	0.3247	**"H22"**	"H"	-17.072	4.436	13.565	0.3247
"N3"	"NC"	4.928	-1.333	5.453	-0.6636	**"N3"**	"NC"	-15.150	4.148	12.800	-0.7313	**"N3"**	"NC"	-15.524	4.938	11.691	-0.7313
"C4"	"CB"	4.674	-1.377	4.118	0.1814	**"C4"**	"CB"	-14.551	3.903	11.611	0.6673	**"C4"**	"CB"	-14.953	5.329	10.520	0.6673
"C3'"	"CT"	4.416	3.378	2.961	0.0713	**"C3'"**	"CT"	-10.340	3.934	11.041	0.2282	**"C3'"**	"CT"	-10.928	4.570	9.949	0.2282
"H3'"	"H1"	4.412	3.941	2.028	0.0985	**"H3'"**	"H1"	-10.958	3.757	10.160	0.1580	**"H3'"**	"H1"	-11.555	5.069	9.211	0.1580
"C2'"	"CT"	5.230	2.096	2.779	-0.0854	**"C2'"**	"CT"	-11.054	3.601	12.336	-0.2099	**"C2'"**	"CT"	-11.691	3.618	10.818	-0.2099
"H2'1"	"HC"	5.668	2.081	1.781	0.0718	**"H2'1"**	"HC"	-11.367	2.562	12.444	0.1718	**"H2'1"**	"HC"	-12.186	2.761	10.359	0.1718

"H2'2"	"HC"	6.025	2.061	3.525	0.0718	**"C32"**	"CT"	-10.089	4.100	13.406	-0.1694	**"C32"**	"CT"	-11.035	3.471	11.692	-0.1694
"O3'"	"OS"	5.030	4.129	3.998	-0.5232	**"O3'"**	"OS"	-9.068	3.331	10.963	-0.6716	**"O3'"**	"OS"	-9.760	3.997	9.406	-0.6716
						"C34"	"CT"	-10.829	4.433	14.699	-0.3219	**"C35"**	"CT"	-10.223	2.215	11.581	-0.3219
						"H35"	"HC"	-9.300	3.370	13.584	0.1168	**"H36"**	"HC"	-9.302	4.444	11.137	0.1168
						"H36"	"HC"	-11.622	5.151	14.489	0.1196	**"H37"**	"HC"	-9.814	4.913	12.624	0.1196
						"H37"	"HC"	-10.132	4.863	15.418	0.1219	**"H38"**	"HC"	-9.668	2.249	10.750	0.1219
						"H38"	"HC"	-11.264	3.524	15.114	0.1239	**"H39"**	"HC"	-9.625	2.133	12.378	0.1239
						"H39"	"HC"	-9.710	6.245	13.344	0.1479	**"H40"**	"HC"	-10.835	1.425	11.541	0.1479
						"H40"	"HC"	-8.445	5.227	12.571	0.1200	**"H41"**	"HC"	-11.604	3.446	12.514	0.1200

Table SIII.21. Atomic charges, atomic names and types for the **native deoxy-C nucleotide** from the standard Amber 94 force field DNA library as implemented in Amber 12[1] with modifications by Pérez *et al.*[4] and for the **modified *7′(R- and S-)*-Me-cLNA-^{Me}C nucleotides** obtained from the HF/6-31G** *ab initio* geometry optimizations performed using GAUSSIAN 03.[5]

Native deoxy-C nucleotide*						***7′R*-Me-cLNA-^{Me}C nucleotide**						***7′S*-Me-cLNA-^{Me}C nucleotide**					
Atom	**Atom Type**	**X**	**Y**	**Z**	**Charge**	**Atom**	**Atom Type**	**X**	**Y**	**Z**	**Charge**	**Atom**	**Atom Type**	**X**	**Y**	**Z**	**Charge**
"P"	"P"	2.314	1.777	-0.478	1.1659	**"P"**	"P"	-9.859	7.089	7.901	1.1660	**"P"**	"P"	-9.027	8.114	8.607	1.1659
"O1P"	"O2"	1.933	3.073	-1.082	-0.7761	**"O1P"**	"O2"	-8.433	6.817	7.619	-0.7373	**"O1P"**	"O2"	-7.681	7.515	8.462	-0.7320
"O2P"	"O2"	3.157	0.872	-1.292	-0.7761	**"O2P"**	"O2"	-10.315	8.480	8.123	-0.7373	**"O2P"**	"O2"	-9.184	9.413	9.298	-0.7320
"O5'"	"OS"	2.994	2.142	0.923	-0.4954	**"O5'"**	"OS"	-10.297	6.208	9.175	-0.6505	**"O5'"**	"OS"	-9.981	7.040	9.332	-0.6618
"C5'"	"CI"	2.156	2.552	2.020	-0.0069	**"C5'"**	"CT"	-9.596	6.308	10.395	0.1250	**"C5'"**	"CT"	-9.706	6.600	10.643	0.1513
"H5'1"	"H1"	1.453	1.754	2.258	0.0754	**"H5'1"**	"H1"	-9.589	7.344	10.734	0.1095	**"H5'1"**	"H1"	-9.684	7.450	11.325	0.1163
"H5'2"	"H1"	1.605	3.450	1.741	0.0754	**"H5'2"**	"H1"	-8.571	5.966	10.249	0.1484	**"H5'2"**	"H1"	-8.740	6.094	10.658	0.1329
"C4'"	"CT"	3.008	2.848	3.243	0.1629	**"C4'"**	"CT"	-10.284	5.431	11.436	0.2378	**"C4'"**	"CT"	-10.798	5.624	11.074	0.2077
"H4'"	"H1"	2.447	3.477	3.934	0.1176	**"C9"**	"CT"	-9.454	5.181	12.693	-0.1978	**"C9"**	"CT"	-10.499	4.874	12.373	-0.2431
"O4'"	"OS"	3.228	1.605	3.977	-0.3691	**"O4'"**	"OS"	-11.520	5.966	11.876	-0.7344	**"O4'"**	"OS"	-12.051	6.256	11.259	-0.7090
"C1'"	"CT"	4.559	1.151	3.778	-0.0116	**"C1'"**	"CT"	-12.272	4.861	12.343	0.5136	**"C1'"**	"CT"	-13.013	5.220	11.177	0.4940
"H1'"	"H2"	5.072	1.095	4.737	0.1963	**"H1'"**	"H2"	-12.649	5.031	13.352	0.1779	**"H1'"**	"H2"	-13.603	5.159	12.091	0.1966
"N1"	"N*"	4.501	-0.268	3.327	-0.0339	**"N1"**	"N*"	-13.382	4.626	11.402	-0.8317	**"N1"**	"N*"	-13.890	5.448	10.014	-0.8376
"C6"	"CM"	4.258	-0.582	2.026	-0.0183	**"C6"**	"CM"	-13.180	4.700	10.055	0.2540	**"C6"**	"CM"	-13.414	6.017	8.868	0.2711
"H6"	"H4"	4.104	0.203	1.300	0.2293	**"H6"**	"H4"	-12.181	4.870	9.679	0.2012	**"H6"**	"H4"	-12.373	6.302	8.811	0.1914
"C5"	"CM"	4.206	-1.878	1.616	-0.5222	**"C5"**	"CM"	-14.215	4.597	9.197	-0.1757	**"C5"**	"CM"	-14.232	6.240	7.819	-0.1888
"H5"	"HA"	4.010	-2.111	0.570	0.1863	**"C17"**	"CT"	-14.006	4.712	7.707	-0.3511	**"C17"**	"CT"	-13.721	6.885	6.553	-0.3165
"C4"	"CA"	4.416	-2.881	2.614	0.8439	**"C4"**	"CA"	-15.517	4.393	9.755	0.6542	**"C4"**	"CA"	-15.601	5.841	7.953	0.6576
"N4"	"N2"	4.379	-4.159	2.286	-0.9773	**"N4"**	"N2"	-16.583	4.302	8.948	-0.7629	**"N4"**	"N2"	-16.453	6.027	6.936	-0.7678
"H41"	"H"	4.532	-4.836	3.019	0.4314	**"H41"**	"H"	-17.504	4.166	9.341	0.3301	**"H41"**	"H"	-17.417	5.739	7.026	0.3428
"H42"	"H"	4.202	-4.434	1.330	0.4314	**"H42"**	"H"	-16.469	4.382	7.948	0.3156	**"H42"**	"H"	-16.130	6.448	6.077	0.3237
"N3"	"NC"	4.653	-2.564	3.884	-0.7748	**"N3"**	"NC"	-15.693	4.298	11.079	-0.7324	**"N3"**	"NC"	-16.047	5.275	9.081	-0.7225
"C2"	"C"	4.701	-1.262	4.273	0.7959	**"C2"**	"C"	-14.641	4.407	11.935	0.9842	**"C2"**	"C"	-15.215	5.066	10.136	0.9748
"O2"	"O"	4.919	-0.928	5.447	-0.6548	**"O2"**	"O"	-14.790	4.335	13.153	-0.6515	**"O2"**	"O"	-15.613	4.554	11.179	-0.6652
"C3'"	"CT"	4.416	3.378	2.961	0.0713	**"C3'"**	"CT"	-10.589	4.007	10.996	0.2181	**"C3'"**	"CT"	-11.074	4.488	10.103	0.2586
"H3'"	"H1"	4.412	3.941	2.028	0.0985	**"H3'"**	"H1"	-11.268	3.965	10.144	0.1329	**"H3'"**	"H1"	-11.431	4.838	9.135	0.1397
"C2'"	"CT"	5.230	2.096	2.779	-0.0854	**"C2'"**	"CT"	-11.278	3.709	12.312	-0.2143	**"C2'"**	"CT"	-12.184	3.955	10.985	-0.2095
"H2'1"	"HC"	5.668	2.081	1.781	0.0718	**"H2'1"**	"H1"	-11.726	2.719	12.396	0.1691	**"H2'1"**	"HC"	-12.736	3.106	10.581	0.1608
"H2'2"	"HC"	6.025	2.061	3.525	0.0718	**"C29"**	"CT"	-10.213	4.031	13.357	-0.1397	**"C29"**	"CT"	-11.465	3.689	12.303	-0.1719

"O3'"	"OS"	5.030	4.129	3.998	-0.5232	**"O3'"**	"OS"	-9.422	3.235	10.817	-0.6645	**"O3'"**	"OS"	-9.993	3.587	10.007	-0.6724
						"H34"	"HC"	-12.945	4.846	7.493	0.1383	**"H31"**	"HC"	-12.647	7.055	6.635	0.1492
						"H35"	"HC"	-14.369	3.807	7.220	0.1240	**"H33"**	"HC"	-14.235	7.834	6.399	0.0959
						"H36"	"HC"	-14.568	5.566	7.330	0.1319	**"H34"**	"HC"	-9.469	4.518	12.381	0.1150
						"H38"	"HC"	-9.552	3.180	13.520	0.1428	**"H35"**	"HC"	-10.708	5.503	13.240	0.1543
						"H39"	"HC"	-9.429	6.065	13.331	0.1306	**"H44"**	"HC"	-13.928	6.231	5.706	0.1393
						"C45"	"CT"	-10.864	4.484	14.662	-0.3207	**"C45"**	"CT"	-10.697	2.372	12.249	-0.3136
						"H40"	"HC"	-8.449	4.858	12.421	0.1380	**"H46"**	"HC"	-10.009	2.387	11.405	0.0868
						"H46"	"HC"	-11.521	5.331	14.462	0.1105	**"H47"**	"HC"	-10.136	2.240	13.174	0.1267
						"H47"	"HC"	-11.446	3.665	15.083	0.1353	**"H48"**	"HC"	-11.400	1.547	12.131	0.1369
						"H48"	"HC"	-10.090	4.786	15.368	0.1128	**"H49"**	"HC"	-12.166	3.697	13.138	0.1542

Table SIII.22. Atomic charges, atomic names and types for the **native deoxy-T nucleotide** from the standard Amber 94 force field DNA library as implemented in Amber 12[1] with modifications by Pérez *et al.*[4] and for the **modified *7'(R- and S-)*-Me-cLNA-T nucleotides** obtained from the HF/6-31G** *ab initio* geometry optimizations performed using GAUSSIAN 03.[5]

Native deoxy-G nucleotide*						***7'R*-Me-cLNA-G nucleotide**						***7'S*-Me-cLNA-G nucleotide**					
Atom	**Atom Type**	**X**	**Y**	**Z**	**Charge**	**Atom**	**Atom Type**	**X**	**Y**	**Z**	**Charge**	**Atom**	**Atom Type**	**X**	**Y**	**Z**	**Charge**
"P"	"P"	2.314	1.777	-0.478	1.1659	**"P"**	"P"	-9.146	8.196	9.035	1.1659	**"P"**	"P"	-9.724	6.992	7.902	1.1659
"O1P"	"O2"	1.933	3.073	-1.082	-0.7761	**"O1P"**	"O2"	-7.784	7.616	9.017	-0.7359	**"O1P"**	"O2"	-8.244	6.989	7.920	-0.7334
"O2P"	"O2"	3.157	0.872	-1.292	-0.7761	**"O2P"**	"O2"	-9.406	9.443	9.789	-0.7359	**"O2P"**	"O2"	-10.457	8.277	7.891	-0.7334
"O5'"	"OS"	2.994	2.142	0.923	-0.4954	**"O5'"**	"OS"	-10.164	7.065	9.560	-0.6482	**"O5'"**	"OS"	-10.241	6.130	9.159	-0.6571
"C5'"	"CI"	2.156	2.552	2.020	-0.0069	**"C5'"**	"CT"	-9.878	6.340	10.735	0.1256	**"C5'"**	"CT"	-9.999	6.572	10.475	0.1344
"H5'1"	"H1"	1.453	1.754	2.258	0.0754	**"H5'1"**	"H1"	-9.888	7.006	11.598	0.1122	**"H5'1"**	"H1"	-10.451	7.553	10.624	0.1133
"H5'2"	"H1"	1.605	3.450	1.741	0.0754	**"H5'2"**	"H1"	-8.889	5.893	10.636	0.1496	**"H5'2"**	"H1"	-8.923	6.642	10.636	0.1452
"C4'"	"CT"	3.008	2.848	3.243	0.1629	**"C4'"**	"CT"	-10.907	5.228	10.923	0.2351	**"C4'"**	"CT"	-10.595	5.577	11.467	0.2272
"H4'"	"H1"	2.447	3.477	3.934	0.1176	**"C9"**	"CT"	-10.491	4.369	11.442	-0.1987	**"C9"**	"CT"	-10.178	5.836	12.914	-0.2076
"O4'"	"OS"	3.228	1.605	3.977	-0.3691	**"O4'"**	"OS"	-12.104	5.643	11.548	-0.7271	**"O4'"**	"OS"	-12.012	5.548	11.445	-0.7180
"C1'"	"CT"	4.559	1.151	3.778	0.0680	**"C1'"**	"CT"	-13.045	4.675	11.138	0.5135	**"C1'"**	"CT"	-12.370	4.262	11.922	0.4620
"H1'"	"H2"	5.072	1.095	4.737	0.1804	**"H1'"**	"H2"	-13.623	4.303	11.984	0.1777	**"H1'"**	"H2"	-13.123	4.319	12.707	0.2140
"N1"	"N*"	4.539	-0.307	3.313	-0.0239	**"N1"**	"N*"	-13.934	5.233	10.103	-0.8514	**"N1"**	"N*"	-12.840	3.440	10.792	-0.8305
"C6"	"CM"	4.317	-0.673	2.011	-0.2209	**"C6"**	"CM"	-13.487	5.424	8.827	0.2321	**"C6"**	"CM"	-12.045	3.236	9.701	0.2495
"H6"	"H4"	4.145	0.084	1.259	0.2607	**"H6"**	"H4"	-12.451	5.218	8.602	0.2071	**"H6"**	"H4"	-11.083	3.726	9.657	0.2037
"C5"	"CM"	4.360	-1.958	1.634	0.0025	**"C5"**	"CM"	-14.304	5.873	7.850	-0.2447	**"C5"**	"CM"	-12.437	2.449	8.676	-0.2156
"C7"	"CT"	4.119	-2.369	0.212	-0.2269	**"C7"**	"CT"	-13.751	6.090	6.462	-0.3106	**"C7"**	"CT"	-11.526	2.272	7.485	-0.3565
"H71"	"HC"	4.860	-1.897	-0.434	0.0770	**"H71"**	"HC"	-12.681	5.882	6.458	0.1432	**"H71"**	"HC"	-11.288	1.215	7.365	0.1798
"H72"	"HC"	4.201	-3.452	0.127	0.0770	**"H72"**	"HC"	-14.260	5.429	5.761	0.1429	**"H72"**	"HC"	-12.034	2.623	6.587	0.1285
"H73"	"HC"	3.120	-2.056	-0.093	0.0770	**"H73"**	"HC"	-13.925	7.124	6.162	0.1171	**"H73"**	"HC"	-10.609	2.842	7.637	0.1264
"C4"	"C"	4.643	-2.997	2.590	0.5194	**"C4"**	"C"	-15.696	6.156	8.117	0.8255	**"C4"**	"C"	-13.715	1.774	8.705	0.8248
"O4"	"O"	4.703	-4.199	2.337	-0.5563	**"O4"**	"O"	-16.510	6.562	7.291	-0.5894	**"O4"**	"O"	-14.148	1.035	7.824	-0.6206
"N3"	"NA"	4.853	-2.538	3.874	-0.4340	**"N3"**	"NA"	-16.078	5.918	9.429	-0.8463	**"N3"**	"NA"	-14.452	2.011	9.856	-0.8229
"H3"	"H"	5.070	-3.289	4.634	0.3420	**"H3"**	"H"	-17.047	6.083	9.663	0.3441	**"H3"**	"H"	-15.345	1.546	9.933	0.3582
"C2"	"C"	4.815	-1.224	4.292	0.5677	**"C2"**	"C"	-15.252	5.464	10.447	1.0709	**"C2"**	"C"	-14.071	2.823	10.914	1.0678
"O2"	"O"	5.015	-0.915	5.455	-0.5881	**"O2"**	"O"	-15.677	5.256	11.581	-0.6327	**"O2"**	"O"	-14.777	2.965	11.910	-0.6479
"C3'"	"CT"	4.416	3.378	2.961	0.0713	**"C3'"**	"CT"	-11.313	4.465	9.661	0.2179	**"C3'"**	"CT"	-10.161	4.128	11.302	0.2476
"H3'"	"H1"	4.412	3.941	2.028	0.0985	**"H3'"**	"H1"	-11.888	5.069	8.960	0.1385	**"H3'"**	"H1"	-10.461	3.707	10.342	0.1143
"C2'"	"CT"	5.230	2.096	2.779	-0.0854	**"C2'"**	"CT"	-12.180	3.575	10.536	-0.2157	**"C2'"**	"CT"	-11.061	3.688	12.441	-0.2293
"H2'1"	"HC"	5.668	2.081	1.781	0.0718	**"H2'1"**	"HC"	-12.790	2.809	10.057	0.1609	**"H2'1"**	"HC"	-11.083	2.616	12.635	0.1502
"H2'2"	"HC"	6.025	2.061	3.525	0.0718	**"C31"**	"CT"	-11.537	3.291	11.370	-0.1407	**"C31"**	"CT"	-10.634	4.558	13.620	-0.1273

"O3'"	"OS"	5.030	4.129	3.998	-0.5232	**"O3'"**	"OS"	-10.240	3.767	9.069	-0.6626	**"O3'"**	"OS"	-8.795	3.935	11.594	-0.6560
						"C33"	"CT"	-12.365	3.233	12.619	-0.3225	**"C33"**	"CT"	-9.489	3.934	14.413	-0.3337
						"H34"	"HC"	-11.086	2.412	11.211	0.1479	**"H34"**	"HC"	-9.094	5.927	12.974	0.1382
						"H35"	"HC"	-12.802	4.119	12.771	0.1109	**"H35"**	"HC"	-10.674	6.718	13.319	0.1417
						"H36"	"HC"	-13.067	2.527	12.520	0.1309	**"H36"**	"HC"	-9.163	4.629	15.186	0.1145
						"H37"	"HC"	-11.778	3.012	13.398	0.1181	**"H37"**	"HC"	-8.658	3.714	13.743	0.1429
						"H38"	"HC"	-10.224	4.567	12.385	0.1330	**"H38"**	"HC"	-9.835	3.011	14.881	0.1002
						"H39"	"HC"	-9.693	4.071	10.917	0.1418	**"H39"**	"HC"	-11.488	4.756	14.270	0.1396

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