Table S1. ^{1}H-NMR chemical shift of O:C duplex (22 ℃ pH 7.0)

residue	H8/H6	AH2/CH5/T-CH$_3$	imino*	amino*		H1'	H2'	H2''	H3'	H4'
G1	7.93					5.98	2.62	2.79	4.84	4.24
T2	7.31	1.39	13.72			5.82	2.14	2.44	4.91	4.13
G3	7.90		12.63			5.57	2.70	2.80	5.02	4.35
A4	8.18	7.78				6.19	2.64	2.88	5.05	4.47
C5	7.09	5.16		6.69	8.08	5.54	1.64	2.16	4.75	4.07
O6	7.92			6.47	6.47	5.73	2.63	2.70	4.96	4.33
C7	7.42	5.41		6.48	8.31	5.58	2.07	2.39	4.84	4.17
A8	8.28	7.73				6.22	2.74	2.88	5.03	4.43
C9	7.32	5.28		6.81	8.1	5.84	1.93	2.42	4.74	4.18
T10	7.30	1.67	14.15			5.83	1.94	2.35	4.84	4.13
G11	7.92		12.91			6.15	2.63	2.30	4.70	4.18
C12	7.64	5.91		7.03	8.24	5.62	1.87	2.36	4.70	4.05
A13	8.30	7.75				6.01	2.81	2.92	5.05	4.39
G14	7.69		12.75			5.92	2.51	2.74	4.94	4.43
T15	7.10	1.34	13.68			5.83	2.01	2.45	4.87	4.21
G16	7.85		12.68			5.74	2.60	2.60	4.96	4.33
C17	7.35	5.27		6.43	9.21	5.92	2.15	2.50	4.84	4.24
G18	7.78		12.77			5.90	2.55	2.75	4.89	4.33
T19	7.26	1.38	13.77			6.01	2.12	2.49	4.86	4.22
C20	7.53	5.69		6.98	8.54	5.54	2.07	2.38	4.84	4.11
A21	8.26	7.82				6.23	2.69	2.88	5.03	4.41
C22	7.29	5.24		6.74	8.18	6.03	2.12	2.12	4.47	3.99

•Chemical shifts at 5 ℃.

Table S2. ^{1}H-NMR chemical shift of O:T duplex (22 ℃ pH 7.0)

residue	H8/H6	AH2/CH5/T-CH$_3$	imino*	amino*		H1'	H2'	H2''	H3'	H4'
G1	7.96					6.00	2.62	2.79	4.83	4.23
T2	7.33	1.39	13.72			5.82	2.13	2.46	4.90	4.21
G3	7.90		12.77			5.58	2.70	2.79	5.02	4.35
A4	8.18	7.78				6.21	2.68	2.91	5.04	4.47
C5	7.19	5.25		6.85	8.21	5.64	1.95	2.36	4.78	4.14
O6	7.85			6.73	6.73	5.80	2.50	2.70	4.94	4.32
C7	7.34	5.36		6.64	8.16	5.58	2.01	2.37	4.83	4.14
A8	8.29	7.70				6.23	2.80	2.91	5.02	4.42
C9	7.32	5.28		6.84	8.11	5.84	1.93	2.43	4.74	4.18
T10	7.23	1.66	14.17			5.83	1.95	2.35	4.85	4.09
G11	7.94					6.17	2.64	2.37	4.70	4.19
C12	7.66	5.94		7.11	8.25	5.64	1.88	2.37	4.71	4.06
A13	8.31	7.76				6.01	2.83	2.92	5.05	4.48
G14	7.71		12.76			5.93	2.52	2.75	4.95	4.43
T15	7.13	1.34	13.58			5.85	2.05	2.48	4.87	4.18
G16	7.83		12.76			6.01	2.51	2.78	4.95	4.38
T17	7.19	1.65	9.18			5.52	2.12	2.31	4.83	4.09
G18	7.88		12.86			5.99	2.63	2.79	4.96	4.37
T19	7.24	1.37	13.75			6.02	2.13	2.51	4.87	4.20
C20	7.53	5.70		6.99	8.55	5.55	2.07	2.39	4.84	4.11
A21	8.29	7.83				6.26	2.70	2.89	5.02	4.41
C22	7.35	5.35		6.64	8.16	6.06	2.12	2.12	4.47	4.01

* Chemical shifts at 5 ℃.

Table S3. ^{1}H-NMR chemical shift of G:C duplex (22 ℃ pH 7.0)

residue	H8/H6	$_{AH2/CH5/T\text{-}CH_3}$	imino*	amino*		H1'	H2'	H2''	H3'	H4'
G1	7.89					5.98	2.64	2.74	4.97	4.24
T2	7.37	1.48	13.7			5.70	2.10	2.44	4.88	4.20
G3	7.94		12.62			5.52	2.72	2.79	5.01	4.35
A4	8.20	7.80				6.21	2.74	2.89	5.05	4.48
C5	7.19	5.21		6.59	8.15	5.55	1.92	2.31	4.80	4.14
G6	7.84		12.86			5.86	2.60	2.71	4.97	4.36
C7	7.33	5.29		6.46	8.33	5.58	2.02	2.39	4.84	4.16
A8	8.28	7.80				6.21	2.74	2.89	5.02	4.42
C9	7.33	5.29		6.82	8.1	5.90	2.02	2.38	4.71	4.12
T10	7.33	1.66	14.15			5.87	2.00	2.42	4.84	4.12
G11	7.88					6.13	2.69	2.36	4.71	4.15
C12	7.70	5.97		7.02	8.23	5.67	1.82	2.39	4.69	4.07
A13	8.30	7.82				6.02	2.79	2.92	5.04	4.40
G14	7.72		12.76			5.94	2.55	2.75	4.93	4.43
T15	7.15	1.35	13.64			5.83	2.07	2.48	4.88	4.20
G16	7.86		12.69			5.87	2.61	2.72	4.98	4.36
C17	7.32	5.39		6.46	8.28	5.68	2.08	2.44	4.84	4.23
G18	7.90		12.86			5.98	2.64	2.74	4.83	4.25
T19	7.25	1.42	13.78			6.01	2.10	2.46	4.84	4.22
C20	7.56	5.73		6.98	8.55	5.44	2.10	2.38	4.84	4.09
A21	8.31	7.85				6.29	2.76	2.85	5.04	4.43
C22	7.34	5.27				6.06	2.15	2.15	4.50	4.02

* Chemical shifts at 5 ℃.

Table S4. ^{1}H-NMR chemical shift of G:T duplex (22 ℃ pH 7.0)

residue	H8/H6	AH2/CH5/T-CH_3	imino*	amino*		H1'	H2'	H2''	H3'	H4'
G1	7.91					5.97	2.60	2.76	4.82	4.22
T2	7.32	1.41	13.72			5.74	2.13	2.44	4.89	4.19
G3	7.90		12.77			5.53	2.69	2.77	5.01	4.34
A4	8.18	7.76				6.20	2.67	2.90	5.04	4.47
C5	7.25	5.28		6.85	8.21	5.67	2.07	2.42	4.79	4.15
G6	7.74					5.90	2.48	2.70	4.91	4.32
C7	7.28	5.36		6.64	8.16	5.53	1.91	2.33	4.81	4.11
A8	8.28	7.70				6.20	2.74	2.89	5.02	4.42
C9	7.31	5.28		6.84	8.11	5.84	1.93	2.43	4.73	4.17
T10	7.29	1.65	14.17			5.84	1.95	2.36	4.82	4.17
G11	7.90					6.14	2.66	2.36	4.69	4.16
C12	7.66	5.94		7.11	8.25	5.63	1.82	2.36	4.69	4.05
A13	8.30	7.76				6.00	2.82	2.92	5.03	4.42
G14	7.71		12.76			5.93	2.51	2.75	4.93	4.42
T15	7.11	1.32	13.58			5.84	2.02	2.46	4.87	4.19
G16	7.82		12.76			6.02	2.52	2.78	4.95	4.39
T17	7.20	1.69	11.62			5.46	2.10	2.26	4.84	4.08
G18	7.94		12.86			6.03	2.68	2.81	4.97	4.36
T19	7.22	1.39	13.75			5.99	2.14	2.47	4.86	4.19
C20	7.53	5.70		6.99	8.55	5.47	2.06	2.35	4.82	4.08
A21	8.29	7.81				6.27	2.73	2.86	5.02	4.41
C22	7.39	5.36		6.64	8.16	6.07	2.15	2.15	4.46	4.01

* Chemical shifts at 5 ℃.

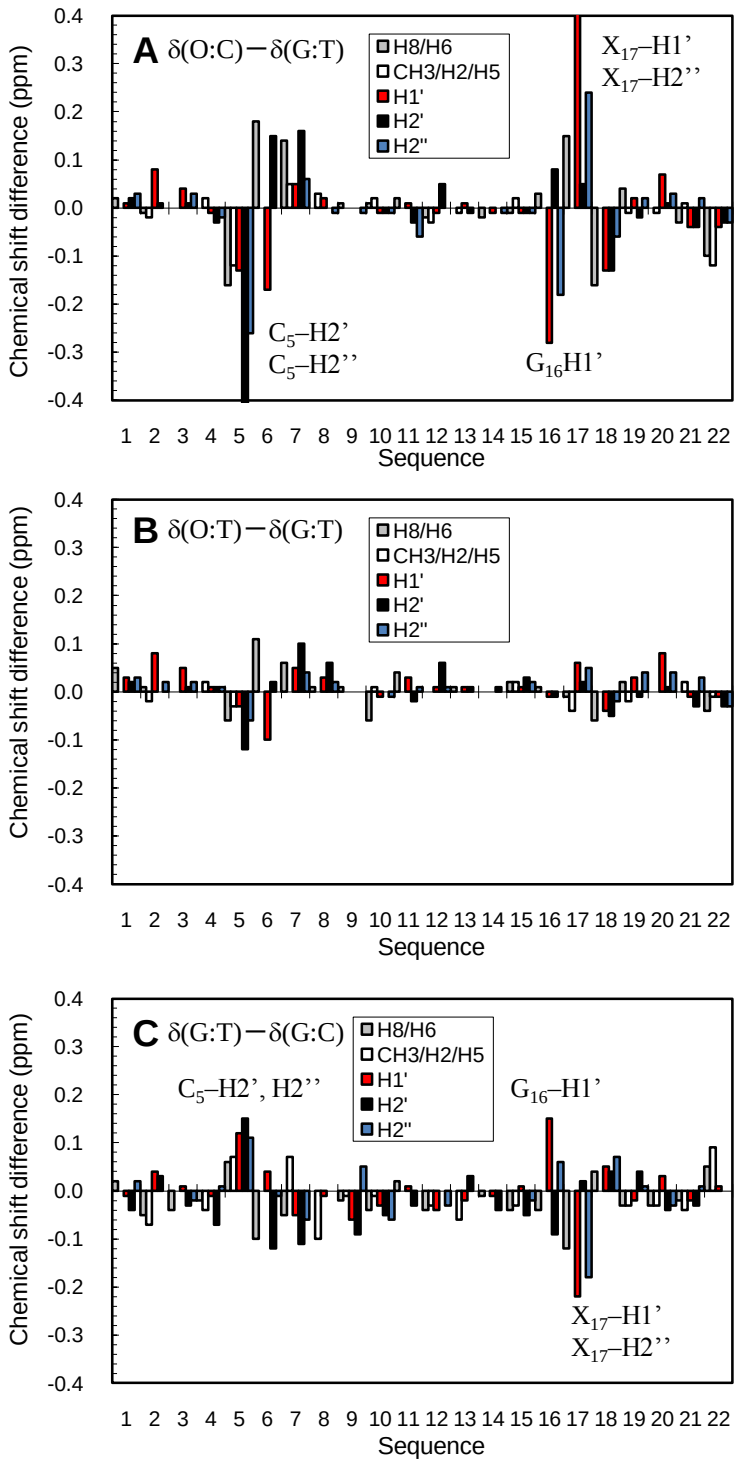

Figure S1. ^{1}H chemical shift differences between the DNA duplexes for H8/H6 (black), T CH_3/A H2/C H5 (white), H1' (red), H2' (gray), H2" (blue): (A) d(O:C duplex) – d(G:T duplex) , (B) d(O:T duplex) – d(G:T duplex), (C) d(G:T duplex) – d(G:C duplex). The protons which showed the large differences between the O:C and O:T duplexes are indicated by the names and sequential numbers..

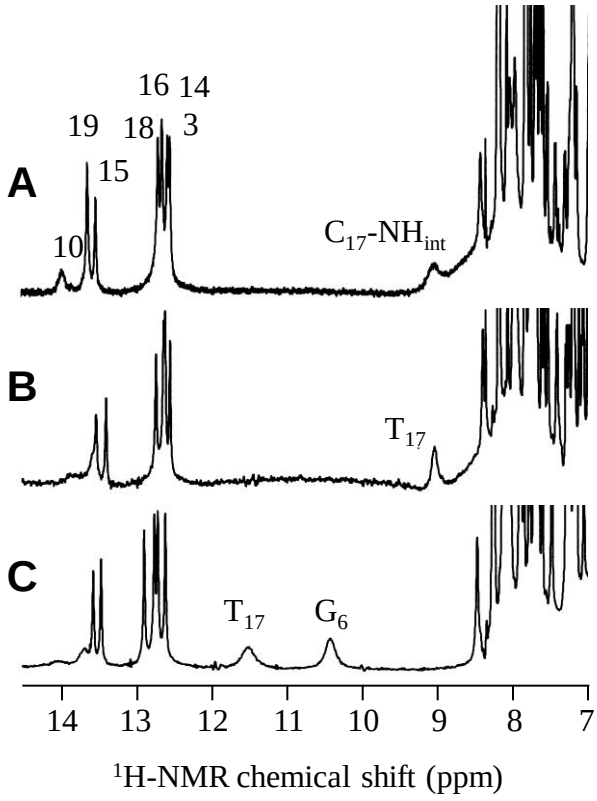

Figure S2. Exchangeable and aromatic proton region of the jump-and return spectra of the mismatched duplexes at pH 7.0, 295 K. (A) O:C, (B) O:T , and (C) G:T duplexes.

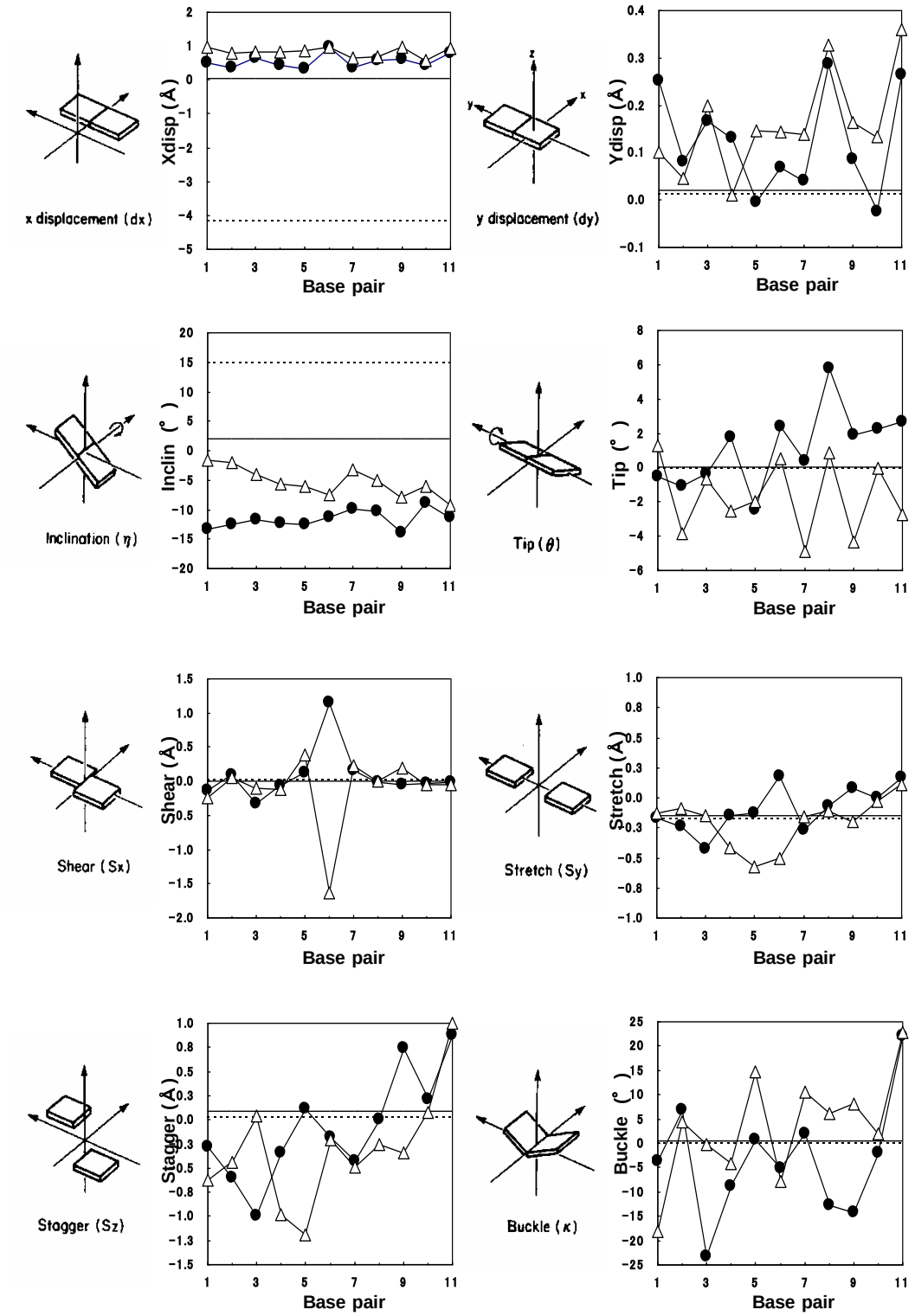

Figure S3. Helical parameters of the O:C (●) and O:T (△) duplexes.
Solid and broken lines indicate typical values of B- and A-DNA, respectively.

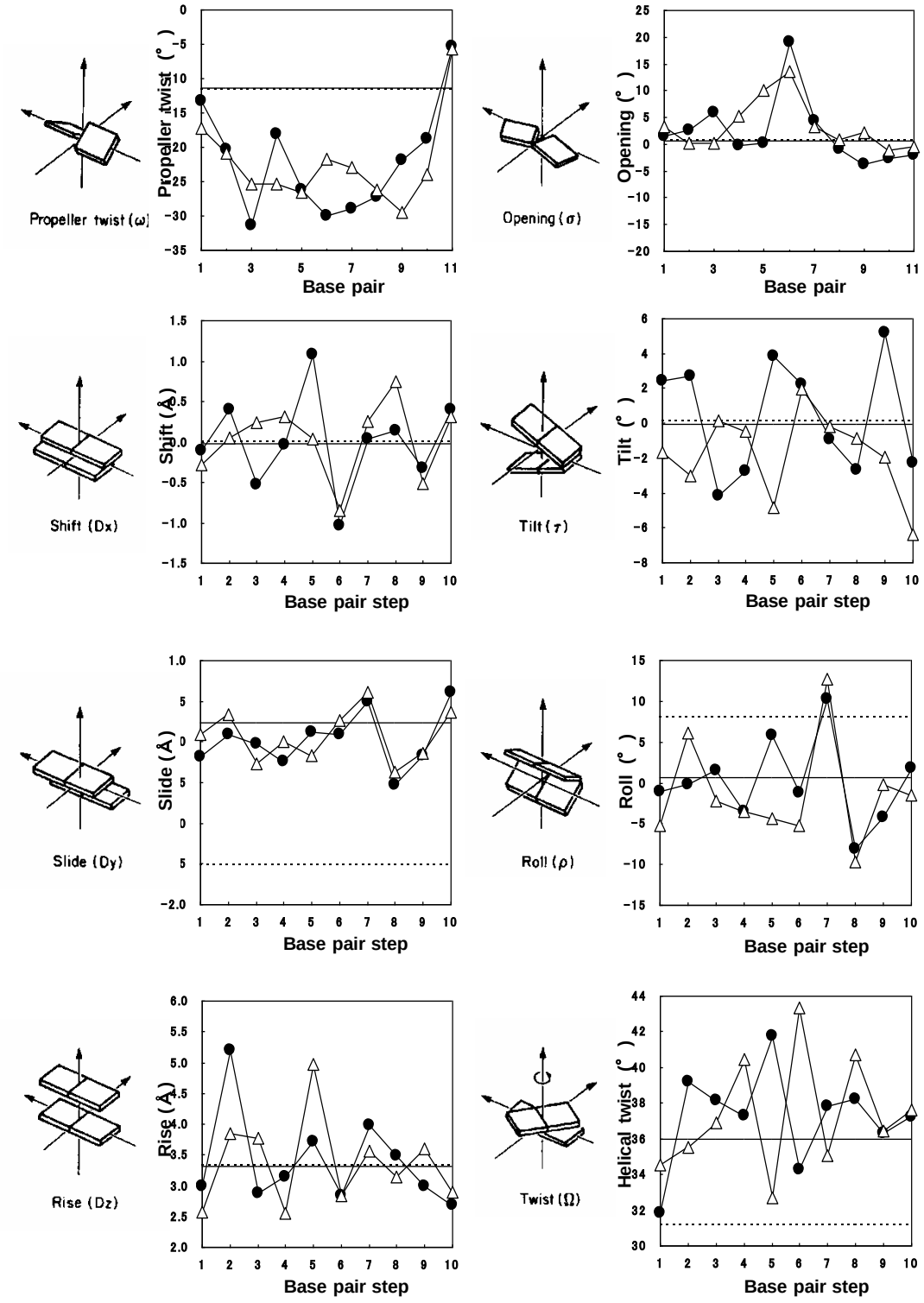

Figure S3. (Continued).

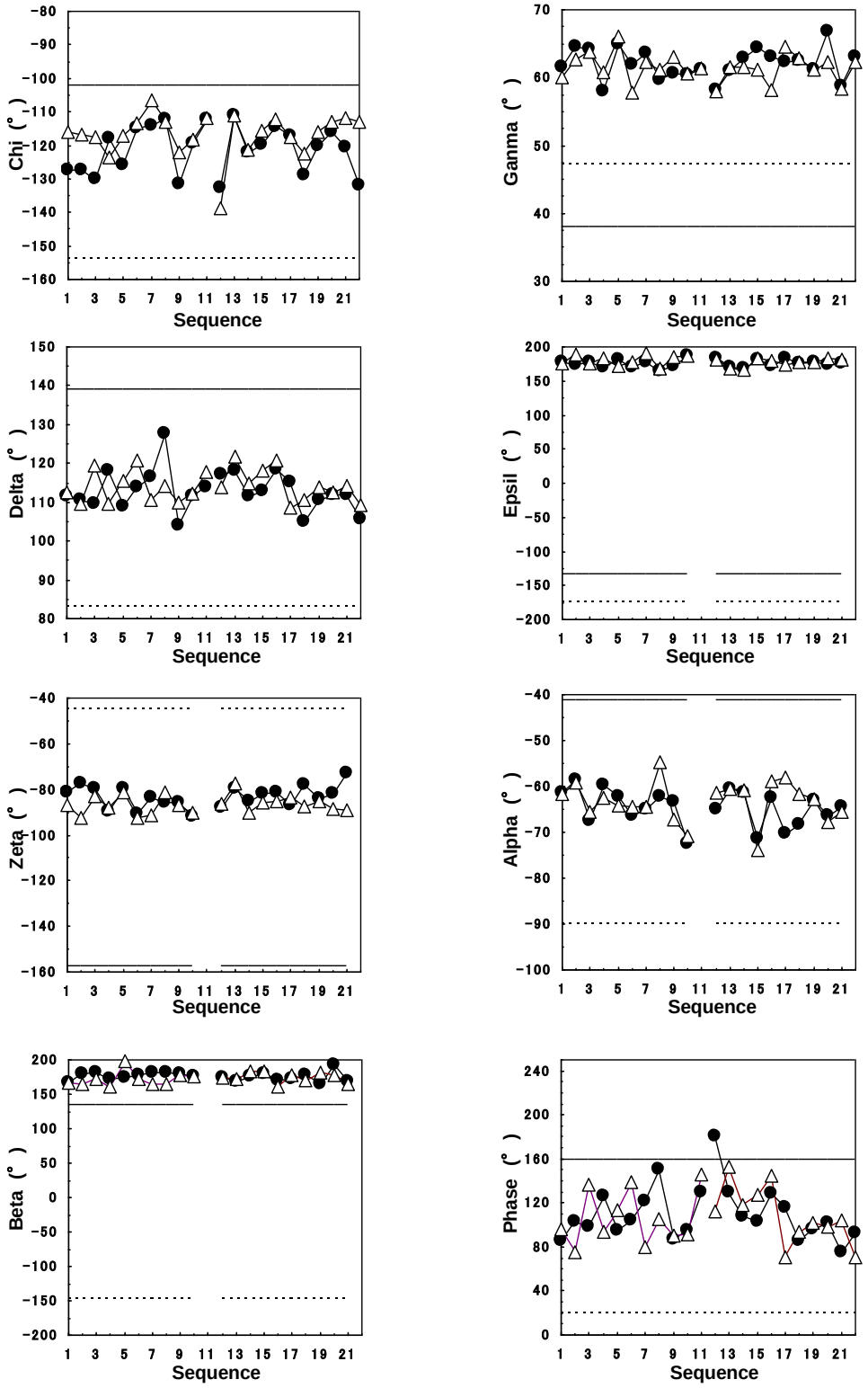

Figure S3. (Continued).