Supplementary tables

Table S1 Molecular dynamics simulation parameters for six systems

System	Number of Na^+ ions	Temperature (K)	Number of atoms	Simulation time (ns)
R2R3 binding with MBS1	6	300	24 574	400
R2R3 binding with MBS1	6	330	24 574	400
Complex F	6	300	24 573	400
Complex F	6	330	24 573	400
Complex R	6	300	24 558	400
Complex R	6	330	24 558	400

R2R3: R2 and R3.

Table S2 Steered molecular dynamics simulation parameters for two systems

System	Number of Na^+ ions	Temperature (K)	Number of atoms	Simulation time (ps)	Pull force (kcal/(mol·nm))
Complex F	6	310	24 573	300	1200
Complex R	6	310	24 558	300	900

Table S3 Summary of RMSDs for five ensembles

Simulation name	Temperature (K)	Time of convergence (ns)	Converged RMSD (nm)
R2R3 binding with MBS1	300	208	0.342
R2R3 binding with MBS1	330	218	0.296
Complex F	300	137	0.267
Complex F	330	158	0.314
Complex R	330	204	0.258

MBS1: Moebius syndrome 1; R2R3: R2 and R3; RMSD: root mean square deviation.

Table S4 Hydrogen-bond interactions of complexes F and R at 330 K

Time (ns)	DNA	Protein	Dist. [Å]
Hydrogen bonds in complex F			
30	A:DT 3[O4]	C:Arg190 [HH12]	2.28
	A:DT 3[O4]	C:Arg190 [HH12]	1.97
	A:DG 7[O6]	C:Lys128 [HZ2]	1.93
50	A:DG 17[O6]	C:Lys182 [HZ1]	1.90
	A:DA 3[H61]	C:Asn183 [OD1]	2.42
	A:DA 4[H61]	C:Asn183 [OD1]	1.97
	A:DG 8[O6]	C:Lys128 [HZ1]	2.00
80	B:DG 27[O6]	C:Lys182 [HZ3]	2.14
	B:DT 28[O4]	C:Lys182 [HZ2]	2.42
	B:DT 29[O4]	C:Arg190 [HH12]	1.77
150	B:DG 27[O6]	C:Lys182 [HZ2]	2.38
	B:DT 28[O4]	C:Lys182 [HZ2]	2.22
	B:DT 29[O5']	C:Arg190 [HH12]	2.28
	B:DA 32[O5']	C:Arg191 [HH22]	1.81
190	A:DC 6[H41]	C:Glu132 [OE1]	1.99
	A:DA 5[O3']	C:Met89 [H2]	2.40
	A:DG 7[O6]	C:Lys128 [HZ2]	2.15
	A:DG 8[O6]	C:Lys128 [HZ1]	1.97
Hydrogen bonds in complex R			
30	A:DA 1[O5']	C:Arg191 [HH22]	1.96
	A:DA 1[O5']	C:Arg191 [HH12]	1.78
	A:DA 1[O4']	C:Arg191 [HH12]	2.30
	A:DG 8[O6]	C:Lys128 [HZ3]	2.39
50	A:DA 3[O5']	C:Asn183 [HD22]	1.90
	A:DG 17[O3']	C:Lys182 [HZ3]	2.42
	A:DG 8[O6]	C:Lys128 [HZ3]	1.97
	A:DT 9[O4]	C:Lys128 [HZ1]	2.00
80	A:DA 1[H62]	C:Ser187 [O]	2.39
	A:DA 3[H61]	C:Ser187 [OG]	2.09
	A:DA 4[H61]	C:Asn183 [OD1]	1.99
150	A:DA 4[H61]	C:Asn183 [OD1]	1.83
	A:DC	C:Glu132	1.80
	A:DC	C:Lys92	2.18
	A:DG	C:Lys128	1.86
190	A:DC	C:Glu132	1.99

Table S5 Hydrogen-bond interactions of complexes F and R in steered molecular dynamics

Time (ns)	DNA	Protein	Dist. [Å]
Hydrogen bonds in complex F			
150	A:DT 1[O5']	C:Arg191 [NH2]	3.06
	A:DT 1[O5']	C:Arg191 [HE]	2.00
	A:DC 6[H41]	C:Arg191 [OE1]	2.05
Hydrogen bonds in complex R			
214	A:DT 1[O4]	C:Arg191 [HH22]	2.43

Supplementary figures

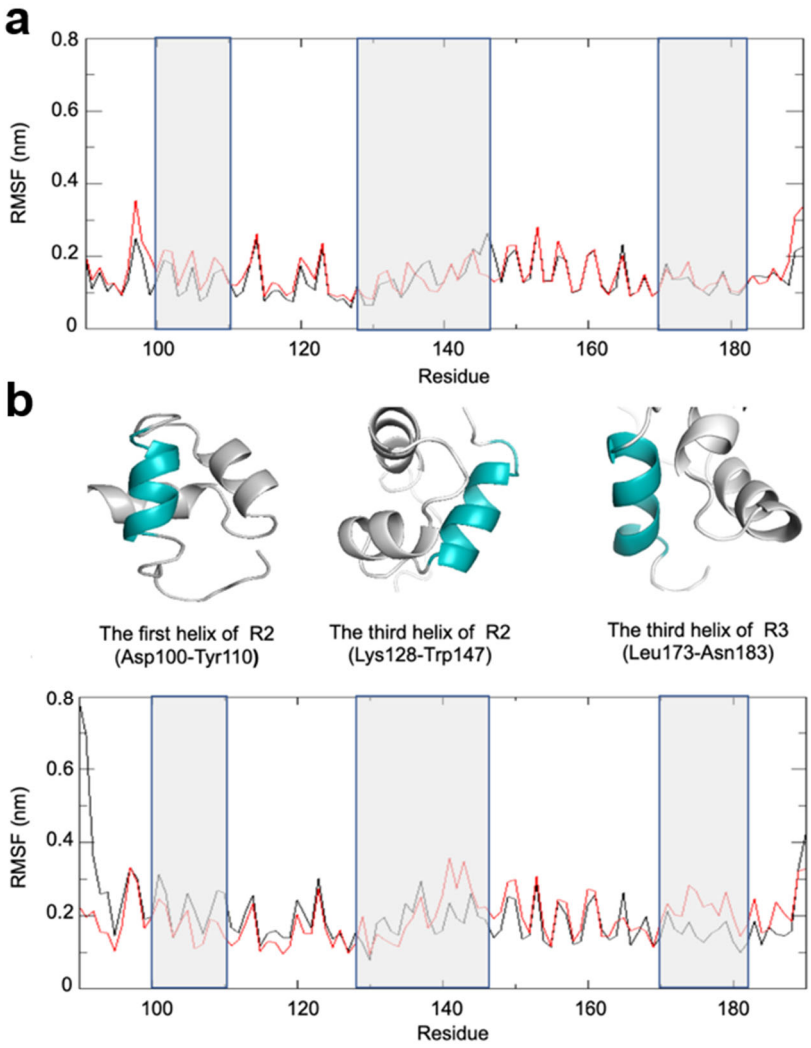

Fig. S1 Root mean square fluctuation (RMSF) profiles. The α-carbon (Cα) atom RMSF per residue is calculated for complexes F and R at 300 K(a) and 330 K (b). Complexes F and R are marked using black and red lines, respectively. Three shade regions correspond to three helices.

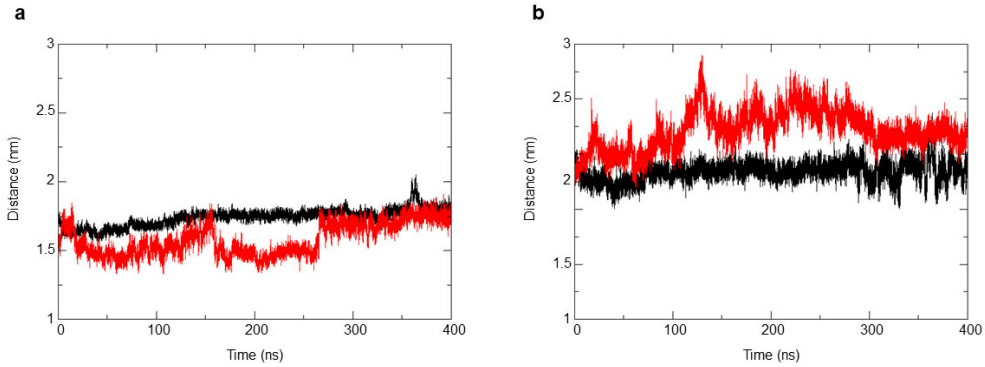

Fig. S2 Distance of recognition helices between R2 and R3 in complexes F and R at 300 K(a) and 330 K (b). Complexes F and R are marked using black and red lines, respectively.

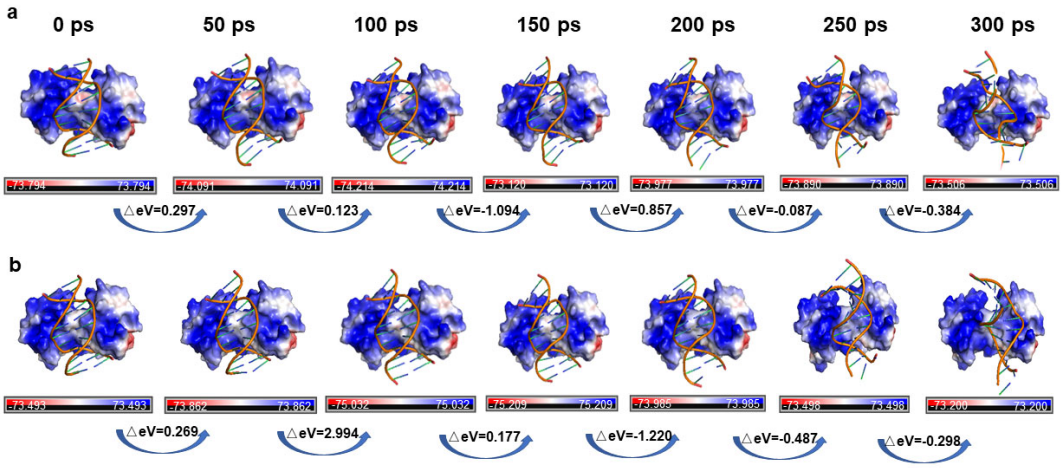

Fig. S3 Electrostatic potential variances of complexes F and R in the steered molecular dynamics (SMD) simulation process. (a) Complex F at 310 K in the 300-ps SMD simulation process; (b) Complex R at 310 K in the 300-ps SMD simulation process.

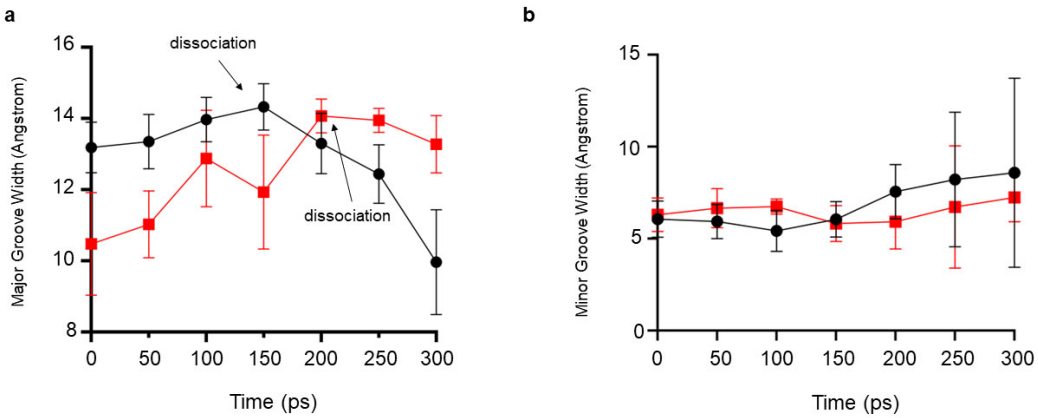

Fig. S4 DNA groove width variances of complexes F and R in the steered molecular dynamics (SMD) simulation process. (a) Major groove width; (b) Minor groove width. Complexes F and R are marked using black and red lines, respectively.