Electronic Supplementary Material (ESI) for Molecular BioSystems.

Table S1.1 Decomposition energy of the DNA molecular. (Kcal·mol^{-1})

	3OSF	K51A	R84A	R87A
C(-3')	0.447	0.381	0.35	0.437
T(-2')	1.215	0.317	1.155	-0.172
G(-1')	1.849	1.374	1.979	-1.902
T(1')	-2.16	0.664	0.454	0.78
A(2')	-2.894	-2.117	-4.581	-4.573
T(3')	-9.27	-4.353	-8.31	-6.424
C(4')	-3.287	-1.118	-0.526	-1.466
G(5')	-5.795	-5.036	0.605	-1.16
T(6')	-0.815	-0.936	0.047	-2.796
C(7')	0.132	0.174	0.235	0.345
T(8')	0.091	0.139	0.193	0.071
T(9')	0.179	0.219	0.266	0.142
G(10')	0.2	0.211	0.228	0.186
C(-4)	0.027	0.135	0.115	0.003
A(-3)	-0.443	-0.255	0.119	0.507
A(-2)	0.86	1.725	1.353	4.448
G(-1)	-0.02	1.399	1.924	-2.284
A(1)	3.597	2.143	2.066	3.458
C(2)	4.137	3.660	1.628	-0.764
G(3)	-7.122	-7.263	-6.524	-6.402
A(4)	0.585	0.502	0.975	0.815
T(5)	-1.493	-2.649	-3.113	-3.169
A(6)	-9.858	-6.465	-6.932	-6.887
C(7)	-3.2	-1.182	-1.893	-1.921
A(8)	0.763	1.057	0.621	0.668
G(9)	0.611	0.486	0.356	0.325
Total	-31.664	-16.788	-17.21	-27.735

Table S1.2 Decomposition energy of the DNA backbone. (Kcal·mol^{-1})

	3OSF	K51A	R84A	R87A
C(-3')	0.328	0.283	0.278	0.294
T(-2')	1.408	0.551	1.586	0.062
G(-1')	1.275	1.884	2.369	-1.18
T(1')	3.268	2.819	2.668	3.177
A(2')	-0.864	2.375	0.23	0.092
T(3')	-3.313	1.045	-0.276	1.011
C(4')	-1.528	0.997	0.137	-0.711
G(5')	0.97	1.249	0.79	0.807
T(6')	0.096	0.119	0.115	0.076
C(7')	0.065	0.104	0.139	0.018
T(8')	0.167	0.221	0.247	0.105
T(9')	0.22	0.264	0.293	0.162
G(10')	0.184	0.197	0.217	0.154
C(-4)	-0.04	0.066	0.042	-0.075
A(-3)	-0.508	-0.29	0.09	0.517
A(-2)	0.705	1.61	1.315	4.609
G(-1)	0.415	1.788	2.217	-0.182
A(1)	3.392	1.924	2.254	3.021
C(2)	4.459	4.243	3.132	0.193
G(3)	-2.618	-2.011	0.05	-0.105
A(4)	0.881	0.885	0.69	0.63
T(5)	0.807	0.222	0.28	0.308
A(6)	-8.208	-5.467	-6.169	-6.112
C(7)	0.088	-0.908	-1.312	-1.293
A(8)	0.798	1.073	0.66	0.668
G(9)	0.62	0.472	0.333	0.343
Total	3.067	15.715	12.375	6.589

Table S1.3 Decomposition energy of the DNA base. (Kcal·mol^{-1})

	3OSF	K51A	R84A	R87A
C(-3')	0.119	0.098	0.072	0.142
T(-2')	-0.193	-0.234	-0.431	-0.235
G(-1')	0.574	-0.51	-0.39	-0.721
T(1')	-5.429	-2.156	-2.214	-2.397
A(2')	-2.03	-4.492	-4.811	-4.665
T(3')	-5.957	-5.398	-8.033	-7.435
C(4')	-1.759	-2.115	-0.663	-0.755
G(5')	-6.765	-6.285	-0.184	-1.967
T(6')	-0.911	-1.056	-0.068	-2.872
C(7')	0.067	0.07	0.096	0.327
T(8')	-0.076	-0.082	-0.054	-0.035
T(9')	-0.041	-0.044	-0.027	-0.02
G(10')	0.016	0.014	0.011	0.032
C(-4)	0.066	0.068	0.073	0.078
A(-3)	0.064	0.035	0.029	-0.009
A(-2)	0.155	0.115	0.039	-0.161
G(-1)	-0.435	-0.389	-0.292	-2.102
A(1)	0.205	0.219	-0.188	0.437
C(2)	-0.323	-0.583	-1.504	-0.957
G(3)	-4.504	-5.252	-6.574	-6.297
A(4)	-0.297	-0.383	0.285	0.185
T(5)	-2.301	-2.871	-3.393	-3.476
A(6)	-1.651	-0.998	-0.763	-0.774
C(7)	-3.289	-0.274	-0.581	-0.628
A(8)	-0.035	-0.017	-0.039	0
G(9)	-0.009	0.014	0.024	-0.019
Total	-34.739	-32.506	-29.58	-34.324

Table S2.1 Decomposition energy of the important residues in 3OSF system (Kcal·mol^{-1})

Residue	Van der Waal	Electrostatic polar	Polar solvation	Non-polar solv	Total
LYS 49	-8.099 +/- 1.274	-324.022 +/- 5.964	323.567 +/- 4.801	-1.285+/-0.063	-9.838 +/- 9.255
GLN 50	-2.213 +/- 1.723	2.674 +/- 5.395	-3.963 +/- 3.591	-0.123+/-0.131	-3.624 +/- 7.786
LYS 51	-5.175 +/- 1.412	-304.378 +/- 7.123	304.665 +/- 6.013	-1.017+/-0.108	-5.905 +/-10.630
LYS72	-0.349 +/- 1.051	-219.688 +/- 8.631	217.332 +/- 7.894	-0.382+/- 0.110	-3.087 +/- 12.656
ARG84	-3.635 +/- 1.538	-293.138+/- 2.155	294.351 +/- 9.213	-0.898+/-0.091	-3.320 +/- 16.461
GLN85	-0.800 +/- 1.633	-13.849 +/- 3.754	8.111 +/- 1.625	-0.239+/-0.048	-6.778 +/- 6.066
ARG87	-2.740 +/- 1.368	-270.383 +/- 9.842	265.887 +/- 8.071	-0.623+/-0.069	-7.859 +/- 14.042
ARG89	-1.579 +/- 1.618	-252.728 +/- 8.762	244.916 +/- 6.353	-0.250+/-0.054	-9.641 +/- 12.460
LYS91	-0.741 +/- 1.453	-267.053+/-11.123	264.600 +/- 10.679	-0.415+/- 0.113	-3.610 +/- 16.168
ARG120	-2.184 +/- 1.266	-257.916 +/- 7.002	251.568 +/- 4.890	-0.479+/-0.139	-9.011 +/- 10.391
GLN121	-0.947 +/- 1.296	-6.207 +/- 4.191	3.271 +/- 2.981	-0.079+/-0.073	-3.962 +/- 6.766
TRP122	-2.688 +/- 1.415	-18.715 +/- 2.343	12.923 +/- 1.262	-0.204+/-0.057	-8.684 +/- 5.827
ALA123	-1.777 +/- 0.891	-9.207 +/- 3.978	6.885 +/- 2.340	-0.397+/-0.089	-4.495 +/- 5.646
ASN139	-3.435 +/- 1.173	-4.455 +/- 3.916	4.183 +/- 2.400	-0.677+/-0.044	-4.384 +/- 6.388
ASN146	-1.256 +/- 0.991	-14.101 +/- 4.716	12.513 +/- 3.070	-0.428+/-0.072	-3.273 +/- 7.110

Table S2.2 Decomposition energy of the important residues in K51A system.

(Kcal·mol^{-1})

Residue	Van der Waal	Electrostatic polar	Polar solvation	Non-polar solv	Total
LYS49	-6.980+/-1.198	-329.905+/-6.749	327.781+/- 5.947	-1.355+/-0.056	-10.458+/-10.361
ALA51	-1.267+/-0.890	-9.391+/- 3.526	5.847+/- 1.768	-0.238+/-0.077	-5.049+/- 5.239
ARG81	-0.338+/-1.980	-232.381+/- 8.955	229.578+/-5.980	-0.001+/-0.048	-3.142+/-12.611
ARG84	-3.849+/-1.380	-295.634+/- 8.218	296.935+/- 5.983	-0.905+/-0.068	-3.454+/- 1.779
GLN85	-0.669+/-1.384	-15.256+/- 3.156	9.334+/- 1.466	-0.185+/-0.049	-6.776+/- 5.349
ARG87	-3.012+/-1.364	-271.462+/- 8.101	266.930+/- 5.882	-0.629+/-0.066	-8.172+/-11.610
ARG89	-0.986+/-1.647	-252.086+/- 8.517	244.639+/- 5.235	-0.235+/-0.053	-8.667+/-11.614
LYS91	-1.351+/-1.292	-279.153+/-10.267	276.788+/- 9.752	-0.511+/-0.130	-4.228+/-14.973
ARG120	-2.083+/-1.225	-257.362+/- 6.947	250.711+/- 5.046	-0.480+/-0.128	-9.215+/-0.371
GLN121	-0.991+/-1.252	-6.080+/- 4.771	2.943+/- 3.605	-0.100+/-0.071	-4.228+/- 7.394
TRP122	-2.800+/-1.326	-18.613+/- 2.556	12.954+/- 1.266	-0.209+/-0.055	-8.668+/- 5.741
ALA123	-1.668+/-0.829	-9.164+/- 2.293	7.009+/-1.629	-0.394+/-0.086	-4.217+/- 4.404
ILE135	-2.409+/-1.443	0.704+/- 2.414	-0.981+/- 0.888	-0.341+/-0.043	-3.027+/- 5.099
ASN139	-3.194+/-1.035	-4.845+/- 3.499	3.772+/- 1.621	-0.625+/-0.039	-4.892+/- 5.833
ASN146	-1.176+/-1.194	-12.334+/-4.557	10.543+/- 3.536	-0.423+/-0.095	-3.390+/- 7.439

Table S2.3 Decomposition energy of the important residues in R84A system.

(Kcal·mol^{-1})

Residue	Van der Waal	Electrostatic polar	Polar solvation	Non-polar solv	Total
LYS49	-6.731+/- 1.195	-324.232+/- 6.969	323.913+/- 5.583	-1.362+/-0.064	-8.413+/- 0.318
LYS51	-3.885+/- 1.050	-271.036+/- 9.580	270.113+/- 9.214	-0.745+/-0.155	-5.553+/-14.367
GLN85	-1.023+/- 1.538	-13.391+/- 3.297	8.378+/- 1.535	-0.323+/-0.088	-6.359+/-5.758
ARG87	-2.867+/- 1.308	-274.318+/- 8.189	269.560+/- 6.250	-0.645+/-0.087	-8.269+/-11.924
ASP88	-1.143+/- 1.346	274.470+/-11.600	-269.831+/- 5.365	-0.212+/-0.073	3.284+/-14.776
ARG89	-1.418+/- 1.849	-250.652+/- 8.309	242.400+/- 6.726	-0.228+/-0.056	-9.898+/- 2.214
LYS91	-1.602+/- 1.274	-281.378+/-11.720	279.028+/-11.860	-0.554+/-0.128	-4.506+/- 7.302
ARG120	-2.362+/- 1.433	-256.658+/- 8.916	250.759+/- 7.847	-0.486+/-0.136	-8.748+/-13.260
GLN121	-1.364+/- 1.261	-5.774+/- 4.376	2.424+/- 3.147	-0.126+/-0.082	-4.839+/- 7.141
TRP122	-2.795+/- 1.334	-20.062+/- 3.111	14.715+/- 1.316	-0.235+/-0.032	-8.376+/- 6.175
ALA123	-1.484+/- 0.742	-10.353+/- 2.495	7.811+/- 1.850	-0.361+/-0.073	-4.387+/- 4.514
ASP134	-1.203+/- 1.310	267.164+/- 9.347	-262.681+/- 8.014	-0.144+/-0.083	3.136+/-13.287
LYS138	-3.084+/- 1.174	-305.716+/- 5.631	312.663+/- 5.082	-0.635+/-0.044	3.228+/- 8.965
ASN139	-3.274+/- 1.085	-3.309+/- 3.224	2.548+/- 1.431	-0.602+/-0.047	-4.636+/- 5.658

Table S2.4 Decomposition energy of the important residues in R87A system.

(Kcal·mol^{-1})

Residue	Van der Waal	Electrostatic polar	Polar solvation	Non-polar solv	Total
LYS49	-6.819+/- 1.261	-320.894+/- 6.621	321.411+/- 6.028	-1.406+/-0.066	-7.707 +/- 10.331
LYS51	-3.720+/- 0.984	-271.460+/-7.918	269.870+/- 7.149	-0.728+/-0.137	-6.039+/- 12.046
GLN85	-0.967+/- 1.508	-14.580+/- 2.826	9.795+/- 1.444	-0.329+/-0.068	-6.081+/- 5.339
ARG89	-1.053+/- 1.929	-243.451+/- 7.796	235.444+/- 5.218	-0.228+/-0.053	-9.288+/- 11.133
HIE100	-1.080+/- 1.930	-13.500+/- 4.836	11.556+/- 3.259	-0.231+/-0.196	-3.255+/- 7.528
ARG120	-1.466+/- 1.366	-254.426+/- 7.606	247.284+/- 5.599	-0.417+/-0.140	-9.025+/- 11.152
TRP122	-2.013+/- 1.437	-16.055+/- 2.534	12.882+/- 1.249	-0.229+/-0.045	-5.415+/- 5.754
LYS138	-2.665+/- 1.094	-297.751+/- 5.734	304.324+/- 5.556	-0.592+/-0.043	3.317+/- 9.348
ASN139	-3.046+/- 1.160	-3.664+/- 4.407	2.175+/- 1.736	-0.531+/-0.045	-5.065+/- 6.620
THR143	-2.627+/- 1.958	-0.197+/- 4.493	0.160+/- 2.541	-0.399+/-0.075	-3.064+/- 7.314
ASN146	-1.374+/- 1.515	-12.879+/- 4.371	9.124+/- 2.460	-0.410+/-0.093	-5.539+/- 6.932
LYS147	-0.197+/- 1.655	-231.030+/- 7.855	224.470+/- 6.594	-0.166+/-0.102	-6.924 +/- 11.461

Figure.S1 The important hydrogen bonds between tvMyb2 and ap65-1 in 3OSF system.