

S2 Table. Hydrogen bonds observed in the GAATTC site during molecular dynamics simulation of *EcoRI* in a complex with DNA containing G or oxoG at the 1st position of the recognition sequence*

Donor	Acceptor	G			oxoG		
		Mean length, Å	Mean energy, kcal/mol	Occurrence, %	Mean length, Å	Mean energy, kcal/mol	Occurrence, %
Protein–DNA bonds							
N[Lys73]	O1P[G/oxoG1]	3.02	–2.26	99	2.98	–2.36	99
		3.01	–2.36	99	2.95	–2.35	99
Nζ[Lys97]	O1P[A2]	3.07	–2.27	96	3.01	–2.35	99
		3.04	–2.30	64	3.06	–2.31	98
N[His98]	O1P[A3]	3.04	–2.31	92	3.09	–2.23	86
		3.06	–2.28	82	3.08	–2.23	78
N[Gly100]	O2P[T4]	3.11	–2.27	99	3.09	–2.29	99
		3.08	–2.25	98	3.07	–2.29	99
N[Asn125]	O ⁴ [T4]	3.13	–2.20	99	3.10	–2.24	99
		3.07	–2.24	99	3.08	–2.24	99
Nδ2[Asn125]	N7[A2]	3.15	–1.69	73	3.14	–1.72	81
		3.15	–1.66	85	3.12	–1.80	97
N[Ala126]	O ⁴ [T4]	3.05	–2.15	96	3.06	–2.15	96
		3.05	–2.12	90	3.06	–2.14	94
Nη2[Arg129]	O2P[A2]	3.07	–1.94	2	3.07	–2.12	62
		3.08	–2.18	85	3.06	–2.29	98
Nζ[Lys132]	O2P[G/oxoG1]	3.05	–2.27	93	3.14	–2.14	44
		3.03	–2.16	7	3.05	–2.20	80
Nη1[Arg187]	O ⁸ [oxoG1]	n/a [#]	n/a	n/a	2.99	–2.33	99
					3.06	–2.29	99
N ⁶ [A2]	Oδ1[Asn125]	2.95	–2.36	99	3.01	–2.34	99
		3.00	–2.33	99	3.03	–2.31	99
N ⁴ [C6]	O[Ala122]	3.02	–2.29	99	3.04	–2.30	99
		3.04	–2.34	99	3.04	–2.39	99
Watson–Crick bonds							
N1[G/oxoG1]	N3[C(6)]	3.11	–1.92	99	3.06	–1.87	98
		3.05	–1.91	99	3.05	–1.86	98
N ² [G/oxoG1]	O ² [C(6)]	2.98	–2.33	99	3.02	–2.38	99
		2.99	–2.39	100	2.98	–2.39	100
N ⁶ [A2]	O ⁴ [T(5)]	2.93	–2.40	99	2.95	–2.40	99
		2.95	–2.39	99	2.97	–2.39	99
N ⁶ [A3]	O ⁴ [T(4)]	3.07	–2.31	99	3.06	–2.30	99
		3.12	–2.23	99	3.07	–2.27	99
N3[T4]	N1[A(3)]	3.12	–1.87	99	3.17	–1.82	99
		3.08	–1.88	99	3.13	–1.85	99
N3[T5]	N1[A(2)]	3.13	–1.87	99	3.12	–1.86	99
		3.14	–1.86	99	3.14	–1.85	99
N ⁴ [C6]	O ⁶ [G/oxoG(1)]	3.05	–2.35	99	2.96	–2.39	99
		2.95	–2.40	100	2.97	–2.38	99

*The bonds existing in at least one of two half-sites for at least 90% of the simulation are listed. The values for both half-sites are presented. Indexes in parenthesis refer to the complementary bases.

[#]n/a, not applied