Supplementary Table 1. Tabulation of Arg-Gua Interactions in Selected Protein-DNA Complexes.[a]

PDBID	Arg-Gua Total[b]	all bidentate[c]	bidentate involving $N^{\varepsilon}/N^{\eta 2}$ [d]	N^{ε}-O6/$N^{\eta 2}$-N7 residue(s)[e]
1A0A	2			
1A3Q	2	2		
1A73	1	1		
1AM9	1			
1AWC	2	2	2	376
1BC8	2	2	2	61
1BDT	1			
1BL0	2	1		
1CEZ	2	2		
1CF7	4	1	1	56
1D02	1	1	1	115
1DMU	2			
1DP7	1	1		
1DSZ	1			
1E3O	1	1		
1ECR	1			
1EFA	1			
1F44[f]	1	1	1	259
1F4K	1	1		
1FIU	3	2	2	191, 194
1FOK	2	2	1	
1G38	1			
1G9Z	4	1		
1GDT	1	1		
1GU4	1	1		
1GXP	2			
1H6F	1			
1H9D	3	3		
1HCR	1			
1HLV	1			
1HWT	1	1	1	118
1I7D	1	1	1	
1IAW	3	2	1	
1IGN	3	2		
1K78	3	3	2	391
1KU7	1	1	1	
1L3L	2	1		
1L3S	2			
1LLM	2	2		

1LQ1	2	2	1	
1M5R	1	1		
1MHD	1	1		
1MNN	3	3		
1NKP	3	3		
1NLW	1			
1P4E[g]	1	1	1	281
1P7H	2	2		
1PUF	1	1		
1QPZ	1	1		
1REP	3	1		
1SKN	1	1		
1TC3	1	1		
1TRO	1	1		
1TUP	1	1		
1UBD	1	1		
2CGP	2			
2DRP	2	2		
2IRF	1			
2UP1	1			
6MHT	1	1		
proteins	**60**	**43**	**14**	**9**
residues	**98**	**63**	**18**	**10**

Legend for Supplementary Table 1

[a] Structure library described in Lejeune *et al.,* "Protein-nucleic acid recognition: statistical analysis of atomic interactions and influence on DNA structure." *Proteins 61,* 258-71 (2005).

[b] Occurences of at least one interaction 3.2 Å or closer between Arg N^{ε}, $N^{\eta 1}$, or $N^{\eta 2}$ and Gua O^6 or N^7 atoms in dsDNA.

[c] Occurrences of paired interactions involving any combination of Arg N^{ε}, $N^{\eta 1}$, or $N^{\eta 2}$ with Gua O^6 and N^7 atoms.

[d] Occurrences of paired interactions of Arg N^{ε} and $N^{\eta 2}$ with Gua O^6 and N^7 atoms, including both N^{ε}-O6/$N^{\eta 2}$-N7 and N^{ε}-N7/$N^{\eta 2}$-O6 paired hydrogen bonds.

[e] N^{ε}-O6/$N^{\eta 2}$-N7 paired hydrogen bonds similar to Cre Arg259

[f] Cre recombinase

[g] FLP recombinase

Supplementary Table 2. Tabulation of Carboxylate-Phosphate Interactions in Selected Protein-DNA Complexes.[a]

PDBID	Residue[b]	Protein Description
1BL0	Glu31	MULTIPLE ANTIBIOTIC RESISTANCE PROTEIN (MARA)/DNA COMPLEX
1CEZ	Asp242	T7 RNA POLYMERASE-T7 PROMOTER COMPLEX
1F44[c]	Glu262	CRE RECOMBINASE TRIMER/DNA COMPLEX
1FZP	Glu11	PLEIOTROPIC VIRULENCE REGULATOR SARA/DNA COMPLEX
1GXP	Glu291	PHOB EFFECTOR DOMAIN/PHO BOX DNA
1N6Q	Glu449	HIV-1 REVERSE TRANSCRIPTASE/AZTMP-TERMINATED DNA

[a] Structure library described in Lejeune *et al.,* "Protein-nucleic acid recognition: statistical analysis of atomic interactions and influence on DNA structure." *Proteins 61,* 258-71 (2005).

[b] Interatomic distances of 3.2 Å or closer between Glu or Asp side chain carboxylate oxygen atoms $O^{\delta 1}$, $O^{\delta 2}$, $O^{\varepsilon 1}$ or $O^{\varepsilon 2}$ and DNA nucleotide phosphate oxygen atoms O^{1P} or O^{2P} in dsDNA.

[c] Cre recombinase

List of 139 selected PDB files from Lejeune *et al.,* "Protein-nucleic acid recognition: statistical analysis of atomic interactions and influence on DNA structure." *Proteins 61,* 258-71 (2005).

1A0A.pdb, 1A1V.pdb, 1A3Q.pdb, 1A73.pdb, 1AIS.pdb, 1AM9.pdb, 1AWC.pdb, 1B01.pdb, 1B3T.pdb, 1BC8.pdb, 1BDT.pdb, 1BG1.pdb, 1BL0.pdb, 1BPY.pdb, 1BRN.pdb, 1C8C.pdb, 1CEZ.pdb, 1CF7.pdb, 1CKT.pdb, 1CL8.pdb, 1CW0.pdb, 1D02.pdb, 1DC1.pdb, 1DDN.pdb, 1DEW.pdb, 1DFM.pdb, 1DH3.pdb, 1DIZ.pdb, 1DMU.pdb, 1DP7.pdb, 1DSZ.pdb, 1E3O.pdb, 1ECR.pdb, 1EFA.pdb, 1EGW.pdb, 1ESG.pdb, 1EWN.pdb, 1EWQ.pdb, 1EXJ.pdb, 1EYG.pdb, 1F0V.pdb, 1F44.pdb, 1F4K.pdb, 1FIU.pdb, 1FOK.pdb, 1FZP.pdb, 1G38.pdb, 1G9Z.pdb, 1GDT.pdb, 1GT0.pdb, 1GU4.pdb, 1GXP.pdb, 1H6F.pdb, 1H9D.pdb, 1HAO.pdb, 1HCR.pdb, 1HI0.pdb, 1HLV.pdb, 1HWT.pdb, 1I3J.pdb, 1I6J.pdb, 1I7D.pdb, 1I8M.pdb, 1IAW.pdb, 1IC8.pdb, 1IGN.pdb, 1J1V.pdb, 1J75.pdb, 1JB7.pdb, 1JE8.pdb, 1JEY.pdb, 1JFI.pdb, 1JJ4.pdb, 1JMC.pdb, 1JT0.pdb, 1JX4.pdb, 1K3X.pdb, 1K4T.pdb, 1K78.pdb, 1KC6.pdb, 1KDH.pdb, 1KU7.pdb, 1KX5.pdb, 1L3L.pdb, 1L3S.pdb, 1LLM.pdb, 1LMB.pdb, 1LQ1.pdb, 1LRR.pdb, 1LWY.pdb, 1M07.pdb, 1M5R.pdb, 1MHD.pdb, 1MJO.pdb, 1MNN.pdb, 1MUS.pdb, 1MW8.pdb, 1MWI.pdb, 1N6Q.pdb, 1NH2.pdb, 1NKP.pdb, 1NLW.pdb, 1NOY.pdb, 1ODH.pdb, 1OE4.pdb, 1ORN.pdb, 1OUP.pdb, 1P4E.pdb, 1P71.pdb, 1P7H.pdb, 1PUF.pdb, 1PV4.pdb, 1QNA.pdb, 1QPI.pdb, 1QPZ.pdb, 1QRV.pdb, 1QUM.pdb, 1R2Z.pdb, 1REP.pdb, 1SKN.pdb, 1T7P.pdb, 1TC3.pdb, 1TRO.pdb, 1TUP.pdb, 1UBD.pdb, 1VAS.pdb, 1ZME.pdb, 2BOP.pdb, 2BPA.pdb, 2CGP.pdb, 2DRP.pdb, 2HDD.pdb, 2IRF.pdb, 2PJR.pdb, 2UP1.pdb, 3HTS.pdb, 3PVI.pdb, 6CRO.pdb, 6MHT.pdb.