

Table 1S. Number of water molecules in the minor groove, major groove and phosphates along the DNA basepairs of the cognate (**BHM_GS**) and non-cognate (**ESG_GS**) complex in the first two solvation shells (up to 5.5 Å).

	Major groove		Minor groove		Phosphate strand 1		Phosphate strand 2		Total	
	BHM_GS	ESG_GS	BHM_GS	ESG_GS	BHM_GS	ESG_GS	BHM_GS	ESG_GS	Σ(BHM)	Σ(ESG)
GC2 (P2,P15)	2.5	11.8	7.8	11.5	0.0	3.1	7.6	12.4	17.9	38.8
GC3 (P3,P14)	2.9	7.3	7.4	8.2	1.5	2.1	12.4	11.5	24.2	29.1
AT4 (P4,P13)	2.0	8.2	1.0	10.5	1.2	0.8	2.8	10.4	7.0	29.9
TA5 (P5,P12)	0.1	7.3	2.3	13.6	0.2	1.7	0.0	1.1	2.6	23.7
CG6,TA6 (P6,P11)	4.6	6.0	8.6	10.0	4.4	10.1	0.8	2.3	18.4	28.4
CG7 (P7,P10)	2.2	8.7	3.7	12.0	11.0	11.0	0.7	3.4	17.6	35.1
Σ	14.3	49.3	30.8	65.8	18.3	28.8	24.3	41.1	87.7	185.0