Supplementary Material For

An anti-DNA Antibody Prefers Damaged dsDNA over Native

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Figure S1. (a) Electrostatic interactions observed in ABDNA_TT and ABDNA between the L-His27d ϵ -hydrogen and the oxygen atoms of the thymine (THY) 10 phosphate group in the DNA's A-strand. The *Fab*'s light chain is shown in blue and the heavy chain is shown in red; the DNA's A-strand is in yellow and the B-strand is in orange. The nucleotides and amino acid residues in the contacts are shown using balls and sticks and colored by the chemical elements. The distances between atoms are shown in purple. (b) Interatomic distances between the L-His27d ϵ -hydrogen atom and the oxygen atom of the THY10 phosphate group at the simulation steps (solid line - for ABDNA_TT, dashed line - for ABDNA). (c) Electrostatic interactions between an oxygen atom of the phosphate group of thymine 10 in the A-strand of DNA and a nitrogen atom of the amino group in the *Fab*'s light chain residue His93.

a) A8 and T9 of the DNA A-strand – Tyr32 of the Fab Light chain

b) T9 and T10 of the DNA A-strand – Trp33 of the Fab Heavy chain

Figure S2. Representative stacking interactions observed in ABDNA_TT and ABDNA. The *Fab*'s light chains are shown in blue and the heavy chain is in red. The DNA's A-strand is shown in yellow and the B strand is in orange. The contacting nucleotides and amino acid residues are represented using sticks. The aromatic ring planes are marked by ellipses.

Figure S3. Maps of contacts revealed between the *Fab*'s *light* chain and DNA in ABDNA_TT and ABDNA. Types of interactions: electrostatic in red, stacking in green, hydrogen bonds in blue, other types are shown in black. The color intensity corresponds to the incidence of this type of interaction in a given position (occupancy). Positions of the amino acid residues are shown horizontally against position positions of the nucleotides (shown vertically) for the A- and B-strands of DNA.

Figure S4. Maps of contacts revealed between the *Fab*'s heavy chain and DNA in ABDNA_TT and ABDNA. Types of interactions: electrostatic in red, stacking in green, hydrogen bonds in blue, other types are shown in black. The color intensity corresponds to the incidence of this type of interaction in a given position (occupancy). Positions of the amino acid residues are shown horizontally against position positions of the nucleotides (shown vertically) for the A- and B-strands of DNA.

a)

				<-----FR1-----><-----CDR1-----><-----FR2-----><-----CDR2-----><-----FR3----->	
V	78.0% (78/100)	Query_1	1	DVLMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGV	
	100.0% (100/100)	A18b	1	DIVMTQTPLSLPVTPGQASISCRSSQNIIVSDGKTYLWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGV	
	97.0% (97/100)	3VW3_L	1	DVLMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGV	
	96.0% (95/99)	3IFP_L	1	DVLMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGV	
	94.0% (94/100)	2C7U_L	2	-VLMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGV	
	95.0% (95/100)	1KTR_L	4	DILMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGV	
	96.0% (96/100)	3NZ8_B	1	DVMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGV	
	96.0% (96/100)	2DDQ_L	1	DVLMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGV	
	96.0% (96/100)	3U9U_B	1	DVLMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGV	
	96.0% (96/100)	2R0Z_L	1	DVLMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGV	
	96.0% (96/100)	2R0W_L	1	DVLMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGV	
	96.0% (96/100)	2IPU_L	1	DVLMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGV	
	96.0% (96/100)	2IPT_L	1	DVLMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGV	
	93.0% (93/100)	3IFO_L	1	DVLMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGI	
	94.0% (94/100)	2IFL_L	1	DVLMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGV	
	94.0% (94/100)	3IFL_L	1	DVLMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGI	
	94.0% (94/100)	4P3C_L	1	DVLMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGV	
	94.0% (94/100)	4OUU_L	1	DVLMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGV	
	93.0% (93/100)	2OJZ_L	1	DILMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGV	
	91.0% (91/100)	2Z4Q_A	1	DILMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGI	
	94.0% (94/100)	4AEI_L	1	DVLMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGV	
	94.0% (94/100)	2DQT_L	1	DVLMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGV	
	93.0% (93/100)	3WFH_B	1	DVLMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGI	
	93.0% (93/100)	3WF6_B	1	DVLMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGI	
	93.0% (93/100)	1FL6_L	1	ELVMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGV	
	94.0% (94/100)	3UTZ_A	1	DVLMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGV	
	95.0% (95/100)	1KEG_L	1	DVLMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGV	
	93.0% (93/100)	2PCP_A	1	DVLMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGV	
	95.0% (95/100)	1EHL_L	1	DVLMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGV	
	93.0% (93/100)	1T9T_L	1	DVLMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGV	
	90.0% (90/100)	1N4X_L	2	DILMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGI	
	92.0% (92/100)	1ZEA_L	1	DVLMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGV	
	92.0% (92/100)	1TET_L	1	DVLMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGV	
	91.0% (91/100)	3NN8_B	2	DIVMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGI	
	94.0% (94/100)	1KEM_L	1	DVLMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGV	
	93.0% (93/100)	4M7J_L	1	DILMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGV	
	93.0% (93/100)	1N0B_A	121	DIELMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGV	
	93.0% (93/100)	4OCX_L	1	DVLMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGV	
	92.0% (92/100)	4HZL_L	1	DVLMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGV	
	91.0% (91/100)	4NKD_B	6	DIVMTQTPLSLPVSLGQASISCRSSQNIIVSNGNTYLEWY LKPGQSPKLLITVKVSNRFSVGPDRFSGSGSGDTFTLKISRVEAEDLGI	

b)

				<-----FR1-----><-----CDR1-----><-----FR2-----><-----CDR2-----><-----FR3----->	
V	65.3% (64/98)	Query_1	1	EVQLQQSGTVLARPASVVKMSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMELSSLTN	88
	100.0% (98/98)	IGHV1-46*03	1	QVQLVQSGAEVKKPGASVKVSCSKASGYFTTISYVIMHWRQAPGQGLEWIGIINPSGGSTSYAQKFGSRVTMTTRDTSTSS--TVYMELSSLRS	88
	91.8% (90/98)	3VW3_H	1	EVQLQQSGTVLARPASVVKMSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMELSSLTN	88
	90.8% (89/98)	300R_H	1	EVQLQQSGTVLARPASVVKMSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMELSSLTN	88
	90.8% (89/98)	1EHL_H	1	EVQLQQSGTVLARPASVVKMSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMEVSSLTN	88
	90.8% (89/98)	1KEG_H	1	EVQLQQSGTVLARPASVVKMSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMEVSSLTN	88
	89.8% (88/98)	3HMS_H	1	EVQLQQSGTVLARPASVVKMSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMEVSSLTN	88
	91.8% (89/97)	3C0D_H	2	-VQLQSQSGTVLARPASVVKMSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMELSSLTN	88
	91.7% (88/96)	1MIM_H	1	--VQLQSQSGTVLARPASVVKMSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMELSSLTN	88
	86.7% (85/98)	1MFA_H	1	EVQLQSQSGTVLARPASVVKMSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMELSSLTN	88
	87.8% (86/98)	3BSZ_H	1	DVLQESGTVLARPASVVKMSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMELSSLTN	88
	89.8% (88/98)	3BGF_H	1	EVQLQESGTVLARPASVVKMSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMELSSLTN	88
	88.8% (87/98)	1MFB_H	1	EVQLQESGTVLARPASVVKMSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMELSSLTN	88
	86.6% (84/97)	1MFA_H	1	EVNLQSGTVLARPASVVKMSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMELSSLTN	88
	78.6% (77/98)	2E27_H	3	QVQLLESQAEALARPASVVKLSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TASQMLSSLAS	90
	80.4% (78/97)	40TX_H	2	-VQLQSQSGAEALARPASVVKLSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMELSSLAS	88
	77.6% (76/98)	3J7E_H	1	EVKLQSGAEALARPASVVKLSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMELSSLAS	88
	76.5% (75/98)	1CTC_B	1	QVQLQQSGELVRPGASVVKLSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMELSSLAS	88
	81.4% (79/97)	4AMK_H	2	-VQLQQSGAEALARPASVVKLSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMELSSLAS	88
	86.2% (81/94)	3IY2_B	1	-----SGTVLARPASVVKMSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMELSSLAS	82
	75.5% (74/98)	2NTE_H	1	QVQLQQSGELVRPGASVVKLSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMELSSLAS	88
	77.6% (76/98)	20SL_H	1	QVQLQQSGAEALARPASVVKMSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMELSSLAS	88
	75.5% (74/98)	1A14_H	1	QVQLQQSGAEALARPASVVKMSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMELSSLAS	88
	75.5% (74/98)	1NMC_H	1	QVQLQQSGAEALARPASVVKMSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMELSSLAS	88
	75.5% (74/98)	1NMA_H	1	EVQLQQSGAEALARPASVVKMSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMELSSLAS	88
	76.5% (75/98)	4DGI_H	1	QVQLQQSGELVRPGASVVKMSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMELSSLAS	88
	74.5% (73/98)	1NMB_H	1	QVQLQQSGAEALARPASVVKMSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMELSSLAS	88
	73.5% (72/98)	1PLG_H	1	QVQLQQSGELVRPGASVVKMSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMELSSLAS	88
	73.5% (72/98)	1T3G_H	1	QVQLQQSGAEALARPASVVKMSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMELSSLAS	88
	73.5% (72/98)	3HBD_A	130	QVQLQQSGELVRPGASVVKMSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMELSSLAS	88
	75.5% (74/98)	4RDO_G	1	QVQLQQSGELVRPGASVVKMSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMELSSLAS	88
	74.5% (73/98)	3UJT_H	1	QVQLQQSGELVRPGASVVKMSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMELSSLAS	88
	76.3% (74/97)	1MRC_H	1	QVQLQQSGAEALARPASVVKMSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMELSSLAS	88
	76.5% (75/98)	2T9L_B	1	QVQLQQSGAEALARPASVVKMSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMELSSLAS	88
	75.5% (74/98)	1TQW_H	1	QVQLQQSGAEALARPASVVKMSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMELSSLAS	88
	78.6% (77/98)	1E6J_H	1	EVQLQQSGAEALARPASVVKMSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMELSSLAS	88
	73.5% (72/98)	400X_H	1	QVQLQQSGELVRPGASVVKMSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMELSSLAS	88
	73.5% (72/98)	1AFV_H	1	QVQLQQSGELVRPGASVVKMSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMELSSLAS	88
	73.5% (72/98)	1JHL_H	1	QVQLQQSGAEALARPASVVKMSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMELSSLAS	88
	76.5% (75/98)	3DGG_B	1	EVKLQQSGELVRPGASVVKMSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMELSSLAS	88
	72.4% (71/98)	3DIF_B	1	EVKLQQSGELVRPGASVVKMSCKASGYFTTINWIMWIKRQPGQGLEWIGTIPGNSDITVYQKFKGAKLTAVTSTSS--TAYMELSSLAS	88

Figure S5. The result of multiple sequence alignments of the light (a) and heavy (b) *Fab*'s chains interacting with different antigens (fragments). Antibodies that are homologous to 64M-5 (44 homologues to the light chain and 56 homologues to the heavy chain) were selected by blasting the NCBI data bank. The canonical CDRs (Kabat et al., 1991) are shown in the upper lines, the aromatic amino acids in CDRs are marked in blue.

Figure S6. Multiple alignment of the light (a) and heavy (b) chains of the 64M-5 antibody's *Fab*-fragment (PDB 3VW3) and homologous sequences from the structures of immune complexes associated with systemic lupus erythematosus (SLE). The MUSCLE algorithm was used (Edgar, 2004). Asterisks show conserved amino acids, red circles represent aromatic amino acids.

Figure S7. Results of the Principal Component Analysis (PCA) for ABDNA and ABDNA_TT. The visual representations of the two first principal components are shown for ABDNA and ABDNA_TT on panels (a) and (b), respectively. The light and heavy chains are shown in blue and red, DNA double helix is in grey and orange, respectively. Two far-most positions in the motion along the PCs are shown as solid and transparent secondary structure elements. The first component (PC1) is the oscillatory motion around a thin part of *Fab* which is marked as a 'hinge'. The second principal components (PC2) are different in the two systems. In ABDNA it corresponds to a motion of *Fab* away from the DNA molecule. In ABDNA_TT it is represented by a shift of the portion of the heavy chain away from the binding interface. Panel (c) shows residue fluctuations along the first PC in ABDNA (black) and ABDNA_TT (blue), the dashed line ellipses indicate the areas of *Fab*'s light and heavy chains that interact with DNA. These areas are numbered 1 through 4 and their respective positions are shown on panels (a) and (b).

Figure S8. Results of the Normal Modes analysis (NMA) for ABDNA and ABDNA_TT. Since the Normal Modes (NMs) are very similar for both systems, only NMs for ABDNA are shown here. Panels (a)-(d) show the motion along normal modes 7 to 10. NMs 7 to 9 correspond to twisting and bending of *Fab* around the hinge region as it is indicated by arrows. NM10 shown on panel (d) correspond to the translational motion of the entire interface away from the DNA molecule. Panel (e) shows the spectrum of normal eigenfrequencies for ABDNA (solid line bars) in comparison with the spectrum of eigenfrequencies for ABDNA_TT (dashed line bars).

Table S1. Relative content¹ of aromatic amino acid residues in the heavy and light chains of the *Fab*-fragments of the antibodies that are homologous to the antibody 64M-5 (see Fig. S5)

Chains	Fraction of aromatic amino acid residues (%)	
	Total amino acid composition	In conserved antigen-binding sites
L	11.7±0.4	15.0±5.1 ²
H	12.0±1.0	16.9±7.1 ²

¹Mean ± standard deviation; ²p<0.05 compared to the total amino acid composition