Two different kinds of interaction modes of deaminase APOBEC3A with single-stranded DNA in solution detected by nuclear magnetic

resonance

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Supplemental figures and tables

Figure S1 Sequence alignment of A3 members indicates the conserved sites for specific identification of target motifs TC and $CC^{1,2}$.





Figure S2 A3A_{4m} is stable for NMR studies within 14 days tested by running ${}^{1}\text{H}{}^{15}\text{N}$ HSQC spectra, in which there was only one set of ${}^{1}\text{H}{}^{15}\text{N}$ cross-peaks.



Figure S3

Figure S3 The ratios of specific complex (*i.e.* S in vertical axis) vs non-specific complex (*i.e.* NS in the abscissa axis) in solution, measured by intensity ratios of the cross-peaks belonging to residues (a) G198, (b) S187, (c) V150 and (d) L12 in HSQC spectra acquired at different molar ratios of TC DNA vs $A3A_{4M}$.



Figure S4 The aggregation states of free A3A_{4M} (in blue) and its complex with TC DNA (in red) determined by ultracentrifugation assay. Based on the fact that the theoretical molecular weights of A3A_{4M} and of free TC DNA are 23.02KDa and 2.99KDa, respectively, we deduced that free A3A_{4M} was a mixture composed by monomer and dimer in solution, but its complex with TC DNA was mainly made of A3A monomer plus TC DNA. In this figure, the complex sample of A3A with DNA was prepared at a molar ratio equal to 2 (TC DNA *vs* A3A).



Figure S5 Chemical shift changes of the protons in two kinds of TC DNA conformers upon it interaction with $A3A_{4M}$. (a) DNA^{S} and (b) DNA^{NS} .



Figure S6 The effects on A3A_{4M} binding affinities by adding bases into 3'- end (*i.e.*, TTC-4 DNA, TTC-5 DNA and TTC-6 DNA) or 5'- end (*i.e.*, TTC-8 DNA, TTC-9 DNA, TTC-10 DNA and TTC-11 DNA), compared to TTC-2. The binding affinities were measured by fluorescent polarization (FP) assay were listed in Table S1.



Figure S7 The base dT_{-1} or dC_{-1} in DNA was specifically identified by the conserved residues in A3 members (shown in figure S1) in different A3-DNA structures. (a) A3A^S-DNA^S complex, (b) A3A-DNA complex (PDB: 5KEG); (c) A3Bctd*-DNA complex (PDB: 5TD5), (d) A3G-CTD2* complex (PDB: 6BUX); In (a-d), DNA sequences were listed in each structure. (e) The conserved residues among A3A, A3B and A3G interact with dT_{-1} or dC_{-1} . The dashed lines represent hydrogen-bonds.



Figure S8 The base dA_{+1} in DNA was specifically identified by the conserved residues in loop 1 of A3 members in different A3-DNA structures. (a) A3A^S-DNA^S complex, (b) A3A-DNA complex (PDB: 5KEG); (c) A3Bctd*-DNA complex (PDB: 5TD5), (d) A3G-CTD2* complex (PDBB: 6BUX); In (a-d), DNA sequences were listed in each structure. (e) The conserved residues in loop 1 among A3A, A3B and A3G interact with dA_{+1} . The dashed lines with stars stands for stacking interactions, while dashed lines without starts represent hydrogen-bonds.



Figure S9 DNA non-specific binding is involved in its interactions with different A3 members. (a) rA3G-CD1 with poly dT ssDNA (PDB: 5K83); (b) hA3F-CD2 dimer with one poly dT ssDNA (PDB: 5W2M); (c and d) hA3Fc-CD2 dimer with one DNA strand containing two TC motifs with PDB codes of 5ZVB and 5ZVA, respectively. The N-and C-termini of A3 proteins, and the 3'- and 5'- ends of DNA were labeled. DNA and A3 proteins were shown in cartoon modes.

Q 184-Ηγ1 Q 184-Ηγ2 A185-β-CH ₃ A185-β-CH ₃ A185-β-CH ₃ A185-β-CH ₃ A185-β-CH ₃ E181-Hα E181-Hβ1 E181-Hβ1 E181-Hβ2 Q184-Hγ1
Q 184-Hγ2 A185-β-CH ₃ A185-β-CH ₃ A185-β-CH ₃ A185-β-CH ₃ A185-β-CH ₃ E181-Hα E181-Hβ1 E181-Hβ2 Q184-Hγ1 Q184-Hγ1
Α185-β-CH ₃ Α185-β-CH ₃ Α185-Hα Α185-β-CH ₃ Α185-β-CH ₃ Ε181-Hα Ε181-Hβ1 Ε181-Hβ1 Ε181-Hβ2 Q184-Hγ1
Α185-β-CH ₃ Α185-β-CH ₃ Α185-β-CH ₃ Α185-Hα Ε181-Hα Ε181-Hβ1 Ε181-Hβ2 Q184-Hγ1
Α185-Ηα Α185-β-CH ₃ Α185-Ηα Ε181-Ηα Ε181-Ηβ1 Ε181-Ηβ2 Q184-Ηγ1
Α185-β-CH ₃ Α185-Ηα Ε181-Ηα Ε181-Ηβ1 Ε181-Ηβ2 Q184-Ηγ1
Α185-Ηα Ε181-Ηα Ε181-Ηβ1 Ε181-Ηβ2 Q184-Ηγ1
Ε181-Ηα Ε181-Ηβ1 Ε181-Ηβ2 Q184-Ηγ1
Ε181-Ηβ1 Ε181-Ηβ2 Q184-Ηγ1
E181-Hβ2 Q184-Hγ1
Q184-Hγ1
0104 11 0
Q184-Hy2
А185-β-СН3
А185-На
А185-На
А185-β-СН3
G25-Hal
G25-Ha2
L186- δ2- CH ₃
Ε181-Ηα
Ε181-Ηβ1
Е181-Нβ2
Η182-Ηα
N24-Ha
I26- δ1-CH ₃
I26- γ2-CH ₃
G25-Ha1
G25-Ha2
I26- δ1-CH ₃
A185-β-CH ₃
G27-Hal
G27-Ha2
I26- δ1-CH ₃
Α185-Ηα
I26- δ1-CH ₃
К30-Нβ1
К30-Нβ2
G25-Hal
G25-Ha2

Table S1 Intermolecular NOEs used in structural determination of A3A^{NS}-DNA^{NS}.

	Ι26- Ηα	
	I26- Нβ	
	I26- γ2-CH ₃	
T5-5-CH3	G25-Hal	
	G25-Ha2	
	Ι26- Ηα	
С6-Н6	I26- HN	
	G27-Hal	
	G27-Ha2	
C6-H5	I26- γ2-CH ₃	
	К30- Нα	
A7-H1'	Q58-Hα	
А7-Н3'	К30- Нβ1	
	К30- Нβ2	
А7-Н4'	Q58-Hα	
	Q58-Hγ1	
	Q58-Hγ2	
А7-Н8	N57- Hβ1	
	Ν57- Ηβ2	
A8-H1'	N57- Hβ1	
	N57- Hβ2	
	Q58- Hβ1	
	Q58- Hβ2	
	F66- Hβ1	
	F66- Нβ2	
A8-H8	А59-β-СН3	
Т9-Н6	L62-Hβ1	
	L62-Hβ1	
	L62- δ1-CH ₃	
T9-5-CH ₃	А59- На	
Т10-Н1'	N63- Hα	

Atom 1 (in DNA ^s)	Atom 2 (in A3A ⁸)		
T2-5-CH ₃	Н182- Нβ1		
	Η182-Ηβ2		
ТЗ-Н1'	I26- δ1-CH ₃		
Т3-Н2'	I26- δ1-CH ₃		
Т3-Н6	I26- γ2-CH ₃		
T3- 5-CH ₃	I26- γ2-CH ₃		
	A185-β-CH ₃		
	L186- δ2-CH ₃		
T4-H1'	I26- γ2-CH ₃		
T4-H6	I26- γ2-CH ₃		
T4- 5-CH ₃	Ι26- Нβ		
	I26- δ1-CH ₃		
	I26- γ2-CH ₃		
Т5-Н6	I26- Нβ		
	I26- γ2-CH ₃		
	W98-Hβ1		
	W98-Hβ2		
	D131- Ηα		
T5- 5-CH ₃	I26- Нβ		
	G27-Hal		
	G27-Hα2		
	W98-Ha		
	Υ132-Нβ1		
	Υ132-Нβ2		
С6-Н1'	Η70-Ηβ1		
	Η70-Ηβ2		
	W98-Ha		
С6-Н2'	N57- Hβ1		
	N57- Hβ2		
С6-Н2"	Τ31-Ηα		
	N57- Hβ1		
	Ν57- Ηβ2		
	Η70-Ηβ1		
	Η70-Ηβ2		
	Р100-Нβ1		
	Р100-Нβ2		
	Ρ100-Ηγ1		
	Ρ100-Ηγ2		
С6-Н3'	Η70-Нδ2		
С6-Н4'	Η29-Ηβ1		
	Н29-Нβ2		

Table S2 Intermolecular NOEs used in structural determination of A3A^s-DNA^s.

	Н70-Нδ2
С6-Н5'	N57- Hβ1
	N57- Hβ2
С6-Н5"	Н29-Нβ1
	Н29-Нβ2
С6-Н6	К30-Нα
	S97-Hβ1
	S97-Hβ2
	W98-Hα
	W98-Hβ1
	W98-Hβ2
	Р100-Нα
	Р100-Нү1
	Р100-Нү2
	С101-Нβ1
	С101-Нβ2
	Υ130- Ηα
С6-Н5	Н70-Нδ2
	H70-Hɛ1
	W98-Hα
	W98-Hδ1
	Р100-На
	Υ130- Ηα
	Υ130- Нδ1
	Ү130- Нб2
	Υ132-Нβ1
	Υ132-Нβ2
A7-H1'	К30-Нα
	R69-Hβ1
	R69-Hβ2
A7-H2'	К30-Нα
	К30-Нβ1
	К30-Нβ2
	Н70-Н82
А7-Н2"	К30-Нα
	K60-Hɛ1
	К60-Нε2
A7-H3'	К30-Нα
	К30-Нβ1
	К30-Нβ2
	К60-Нβ1
	К60-Нβ2
	Κ60-Ηδ1

К60-Н62 К60-Н62 К60-Н62 К60-Н62 К30-Нβ1 К30-Нβ2 А7-Н8 К30-На А59-β-СН3 К60-На2 А8-Н1' К60-На А8-Н2' К60-На К60-На2 К60-На А8-Н2' К60-На1 К60-На2 К60-На1 К60-На2 К60-На1 К60-На2 К60-На1 К60-На2 К60-На1 К60-На2 К60-На1 К60-На1 К60-На2 К60-На2 К60-На1 К60-На3 К60-На1 К60-На4 К60-На1 К60-На5 К60-На2 К60-На5 К60-На2 К60-На5 К60-На5 К60-На5			
К60-Нь1 К60-Нь2 А7-Н5' К30-Нβ1 К30-Нβ2 А7-Н8 К30-На А59-На А59-β-СН3 К60-На К60-На А8-Н1' К60-На А8-Н2' К60-На К60-На2 К60-На К60-На2 К60-На1 К60-На2 К60-На2 А8-Н2' К60-На1 К60-На2 К60-На2 А8-Н3' Q58-Нβ1 Q58-Нβ2 К60-На К60-На2 К60-На Ц62-δ1-СН3 К60-На2 К60-На3 К60-На2 К60-На4 К60-На5 К60-На52 К60-На52 К60-На52 К60-На61 К60-На52 К60-На61 К60-На52 К60-На61 К60-На52 К60-На61 К60-На61 К60-На61 К60-На61 К60-На61 К60-На61 К60-На61 К60-На62 К60-На61 К60-На62 К60-На61 К60-На62		К60-Н82	
К60-Не2 А7-Н5' К30-Нβ1 К30-Нβ2 А7-Н8 К30-На А59-На А59-На А59-β-СН3 К60-На К60-На К60-На А8-Н1' К60-На А8-Н2' К60-На К60-На К60-На А8-Н2' К60-На К60-На К60-На		K60-Hε1	
A7-H5' K30-Hβ1 A7-H8 K30-Hα A59-β-CH ₃ K60-Hα A8-H1' R69- Hα A8-H2' K60-Hε1 K60-Hε2 K60-Hε1 K60-Hε2 K60-Hε1 K60-Hε1 K60-Hε2 A8-H2' K60-Hε1 K60-Hε2 K60-Hε1 K60-Hε2 K60-Hε1 K60-Hε2 K60-Hε1 K60-Hε2 K60-Hε1 K60-Hε2 K60-Hε1 K60-Hε3 K60-Hε3 K60-Hε4 K60-Hε3 K60-Hε3		К60-Нε2	
K30-Hβ2 A7-H8 K30-Hα A59-β-CH ₃ K60-Hα A59-β-CH ₃ K60-Hα A8-H1' R69- Hα A8-H2' K60-Hε1 K60-Hε2 K60-Hε1 K60-Hε1 K60-Hε1 K60-Hε2 K60-Hε1 K60-Hε1 K60-Hε1 K60-Hε2 K60-Hε1 K60-Hε1 K60-Hε1 K60-Hε2 K60-Hα L62-81-CH ₃ K60-Hα K60-Hε1 K60-Hε1 K60-Hε2 K60-Hε1 K60-Hε3 K60-Hε1 K60-Hε1 K60-Hε2 T9-H3' L62-δ1-CH ₃ T9-H3' L62-δ1-CH ₃ K60-Hε1 K60-Hε3 K60-Hε2 K60-Hε1 K60-Hε3 K60-Hε3 K60-Hε1 K60-Hε3 K60-Hε1 K60-Hε3 K60-Hε1 K60-Hε3 K60-Hε2 L62-δ1-CH ₃ L62-Hβ1 L62-Hβ1 L62-Hβ1 L62-Hβ1 L62-A1-CH ₃ <t< th=""><th>A7-H5'</th><th colspan="2">К30-Нβ1</th></t<>	A7-H5'	К30-Нβ1	
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Α59-Hα Α59-β-CH ₃ K60-Hα Λ8-H1' R69-Hα Λ8-H2' K60-Hε1 K60-Hε2 Λ8-H2'' K60-Hε1 K60-Hε1 K60-Hε2 Λ8-H2'' K60-Hε2 Λ8-H2'' K60-Hε1 K60-Hε2 Λ8-H3' Q58-Hβ1 Q58-Hβ2 K60-Hα L62-δ1-CH ₃ Λ8-H8 K60-Hα K60-Hδ1 K60-Hδ2 K60-Hε1 K60-Hε2 T9-H3' L62-δ1-CH ₃ T9-5-CH ₃ K60-Hδ1 K60-Hδ2 K60-Hδ1 K60-Hδ2 K60-Hδ1 K60-Hδ2 K60-Hδ1 K60-Hδ2 K60-Hε1 K60-Hε2 L62-δ1-CH ₃ L62-Hβ1 L62-Hβ2 L62-Hβ2 L62-A1-CH ₃	А7-Н8	К30-Нα	
A59-β-CH3 K60-Hα A8-H1' R69- Hα A8-H2' K60-Hε1 K60-Hε2 K60-Hε3 A8-H2' K60-Hα K60-Hε1 K60-Hε3 A8-H3' Q58-Hβ1 Q58-Hβ2 K60-Hα L62-δ1-CH3 K60-Hα K60-Hε3 K60-Hε3 T9- 5-CH3 K60-Hε3 K60-Hε3 K60-Hε3 K60		Α59-Ηα	
K60-Hα A8-H1' R69- Hα A8-H2' K60-Hε1 K60-Hε2 K60-Hε A8-H2'' K60-Hα K60-Hε2 K60-Hε A8-H3' Q58-Hβ1 Q58-Hβ2 K60-Hα L62-δ1-CH3 K60-Hα A8-H3' K60-Hα L62-δ1-CH3 K60-Hα K60-Hε2 K60-Hα K60-Hε3 K60-Hα K60-Hε3 K60-Hε3 K60-Hε3 K60-Hε3 K60-Hε1 K60-Hε3 T9-H3' L62-δ1-CH3 T9-5-CH3 K60-Hα K60-Hε1 K60-Hε3 K60-Hε3 K60-Hε3		А59-β-СН3	
A8-H1' R69- Hα A8-H2' K60-Hε1 K60-Hε2 K60-Hε1 K60-Hε1 K60-Hε1 K60-Hε2 K60-Hε1 K60-Hε2 K60-Hε1 K60-Hε2 K60-Hε1 K60-Hε2 K60-Hε1 K60-Hε2 K60-Hε1 K60-Hε2 K60-Hε1 K60-Hε3 K60-Hα L62-δ1-CH3 K60-Hδ1 K60-Hε1 K60-Hε1 K60-Hε2 K60-Hε1 K60-Hε1 K60-Hε1 K60-Hε2 K60-Hε1 K60-Hε1 K60-Hε1 K60-Hε2 K60-Hε1 K60-Hε1 K60-Hε1 K60-Hε2 L62-δ1-CH3 T9- 5-CH3 K60-Hε1 K60-Hε1 K60-Hε2 L62- δ1-CH3 L62-Hβ1 L62-Hβ1 L62-Hβ2 L62-Hβ2 L62-Hβ2 L62-δ1-CH3 L62-K1-CH3 L62-δ1-CH3 L62-K1-CH3		Κ60-Ηα	
A8-H2' K60-Hε1 A8-H2'' K60-Hα A8-H2'' K60-Hα K60-Hε2 K60-Hε1 K60-Hε2 K60-Hα A8-H3' Q58-Hβ1 Q58-Hβ2 K60-Hα L62-81-CH3 L62-81-CH3 A8-H8 K60-Hα K60-Hε1 K60-Hε1 K60-Hε2 K60-Hε1 K60-Hε3 K60-Hε1 K60-Hε1 K60-Hε2 T9-H3' L62-δ1-CH3 T9-5-CH3 K60-Hα K60-Hε1 K60-Hε3 K60-Hε1 K60-Hε1 K60-Hε2 L62-δ1-CH3 T9-5-CH3 K60-Hε1 K60-Hε1 K60-Hε3 K60-Hε1 K60-Hε3 K60-Hε1 K60-Hε3 K60-Hε1 K60-Hε3 K60-Hε2 L62-Hα L62-Hβ1 L62-Hβ1 L62-Hβ2 L62-δ1-CH3 L62-δ1-CH3 L62-δ2-CH3	A8-H1'	R69- Ηα	
K60-Hε2 A8-H2'' K60-Hα K60-Hε1 K60-Hε2 A8-H3' Q58-Hβ1 Q58-Hβ2 K60-Hα L62-δ1-CH3 K60-Hα A8-H8 K60-Hα K60-H81 K60-Hα K60-H82 K60-Hα K60-H81 K60-Hα K60-H82 K60-Hα T9-H3' L62-δ1-CH3 T9- 5-CH3 K60-Hα K60-H82 K60-Hα K60-H82 K60-Hα L62-δ1-CH3 K60-Hα L62-δ1-CH3 K60-Hα L62-δ1-CH3 K60-Hα L62-δ1-CH3 K60-Hα2 L62-Hβ1 L62-Hβ2 L62-Hβ1 L62-Hβ1 L62-Hβ1 L62-Hβ2 L62-δ1-CH3 L62-δ1-CH3 L62-δ1-CH3 L62-Hβ2	A8-H2'	K60-Hɛ1	
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К60-Нε1 K60-Нε2 A8-H3' Q58-Hβ1 Q58-Hβ2 K60-Ha L62-81-CH3 L62-81-CH3 A8-H8 K60-Ha K60-Ha1 K60-Ha2 K60-Ha2 K60-Ha1 K60-Ha1 K60-Ha2 T9-H3' L62- 81-CH3 T9- 5-CH3 K60-Ha1 K60-Ha2 K60-Ha1 K60-Ha1 K60-Ha2 T9- 5-CH3 K60-Ha1 K60-Ha2 L62- 81-CH3 K60-Ha2 L62-Ha1 L62-Ha1 L62-Ha2 L62-Hp1 L62-Hp1 L62-Hp2 L62-Hp2 L62- 81-CH3 L62-KB2	A8-H2"	Κ60-Ηα	
K60-Hε2 A8-H3' Q58-Hβ1 Q58-Hβ2 K60-Hα L62-δ1-CH3 L62-δ1-CH3 A8-H8 K60-Hα K60-H82 K60-H82 K60-H22 K60-Hε1 T9-H3' L62-δ1-CH3 T9-H3' L62-δ1-CH3 T9-5-CH3 K60-Hε2 K60-Hε2 K60-Hε3 K60-Hε3 K60-Hε3 K60-Hε3 K60-Hε3 L62-δ1-CH3 K60-Hε3 L62-Hε3 K60-Hε3 L62-Hε3 K60-Hε3 L62-Hε3 L62-Hε3 L62-Hε3 L62-Hε3		K60-Hɛ1	
A8-H3' Q58-Hβ1 Q58-Hβ2 K60-Hα L62-δ1-CH3 L62-δ1-CH3 A8-H8 K60-Hα K60-H81 K60-H82 K60-H82 K60-H82 T9-H3' L62-δ1-CH3 T9-H3' L62-δ1-CH3 T9-5-CH3 K60-Hα K60-H81 K60-Hα K60-H81 K60-Hα L62-δ1-CH3 L62-δ1-CH3 L62-H81 K60-Hα2 L62-Hβ1 L62-Hβ1 L62-Hβ1 L62-Hβ2 L62-δ1-CH3 L62-Hβ2 L62-δ1-CH3 L62-Hβ2		К60-Нε2	
Q58-Hβ2 K60-Hα L62-δ1-CH3 A8-H8 K60-Hα K60-Hδ1 K60-Hε2 K60-Hε2 T9-H3' L62-δ1-CH3 T9-H3' L62-δ1-CH3 K60-Hε1 K60-Hε2 K60-Hε2 K60-Hε3 K60-Hε3 K60-Hε3 K60-Hε3 K60-Hε3 K60-Hε3 K60-Hε3 L62-δ1-CH3 L62-Hε3 L62-Hε3 L62-Hε3 L62-Hε3 L62-Hε3 L62-Hε3 L62-Hε3 L62-Hε3 L62-Hε3	А8-Н3'	Q58-Hβ1	
K60-Hα L62-δ1-CH3 A8-H8 K60-Hα K60-Hδ1 K60-Hδ2 K60-Hε1 K60-Hε2 T9-H3' L62-δ1-CH3 T9-5-CH3 K60-Hα K60-Hδ1 K60-Hα K60-Hδ2 L62-δ1-CH3 T9-5-CH3 K60-Hα K60-Hδ1 K60-Hδ2 L62-δ1-CH3 L62-Hδ1 L62-Hδ1 L62-Hβ2 L62-Hβ1 L62-Hβ2 L62-δ1-CH3 L62-Hβ2 L62-δ1-CH3 L62-CH3		Q58-Hβ2	
L62-δ1-CH₃ A8-H8 K60-Hα K60-Hδ1 K60-Hδ2 K60-Hε1 K60-Hε2 T9-H3' L62- δ1-CH₃ T9-5-CH₃ K60-Hα K60-Hδ1 K60-Hα K60-Hδ1 L62-δ1-CH₃ L62-δ1-CH₃ L62-HΔ L62-δ1-CH₃ L62-HΔ L62-HΔ L62-HΔ L62-HΔ L62-HΔ L62-HΔ L62-HΔ L62-HΔ L62-HΔ L62-HΔ L62-HΔ L62-HΔ L62-HΔ L62-Λ1-CH₃ L62-Λ1-CH₃		Κ60-Ηα	
A8-H8 K60-Hα K60-Hδ1 K60-Hδ2 K60-Hε1 K60-Hε2 T9-H3' L62- δ1-CH ₃ T9- 5-CH ₃ K60-Hα K60-Hδ1 K60-Hδ1 K60-Hδ2 K60-Hδ1 K60-Hδ1 K60-Hδ2 L62-δ1-CH ₃ L62-Hδ1 L62-Hδ2 L62-Hβ1 L62-Hβ1 L62-Hβ2 L62-δ1-CH ₃ L62-K3-CCH ₃		L62-81-CH3	
K60-Hδ1 K60-Hδ2 K60-Hε1 K60-Hε2 T9-H3' L62-δ1-CH ₃ T9- 5-CH ₃ K60-Hδ1 K60-Hδ2 K60-Hδ1 K60-Hδ2 L62-δ1-CH ₃ L62-Hδ1 L62-Hδ2 L62-Hβ1 L62-Hβ1 L62-Hβ2 L62-δ1-CH ₃ L62-CH ₃	A8-H8	Κ60-Ηα	
K60-Hδ2 K60-Hε1 K60-Hε2 T9-H3' L62- δ1-CH ₃ T9- 5-CH ₃ K60-Hδ1 K60-Hδ2 K60-Hδ1 K60-Hδ2 L62-δ1-CH ₃ L62-Hδ1 L62-Hδ2 L62-Hβ1 L62-Hβ2 L62-δ1-CH ₃ L62-δ1-CH ₃		К60-Нδ1	
K60-Hε1 K60-Hε2 T9-H3' L62- δ1-CH ₃ T9- 5-CH ₃ K60-Hα K60-Hδ1 K60-Hδ2 K60-Hε1 K60-Hε2 L62-A L62-Hα L62-Hβ1 L62-Hβ2 L62-δ1-CH ₃ L62-Hβ2 L62-δ1-CH ₃ L62-CH ₃		К60-Нδ2	
K60-Hε2 T9-H3' L62- δ1-CH ₃ T9- 5-CH ₃ K60-Hα K60-Hδ1 K60-Hδ2 K60-Hε1 K60-Hε2 L62-Hα L62-Hβ1 L62-Hβ2 L62-Hβ1 L62-δ1-CH ₃ L62-Hβ2		K60-Hɛ1	
T9-H3' L62- δ1-CH ₃ T9- 5-CH ₃ K60-Hα K60-Hδ1 K60-Hδ2 K60-Hε1 K60-Hε2 L62-Hα L62-Hβ1 L62-Hβ1 L62-Hβ2 L62-δ1-CH ₃ L62-CH ₃		К60-Нε2	
T9- 5-CH ₃ K60-Hα K60-Hδ1 K60-Hδ2 K60-Hε1 K60-Hε2 L62-Hα L62-Hβ1 L62-Hβ2 L62-Aβ2 L62-Aβ2 L62-CH ₃	Т9-Н3'	L62- δ1-CH ₃	
K60-Hδ1 K60-Hδ2 K60-Hε1 K60-Hε2 L62-Hα L62-Hβ1 L62-Hβ2 L62-δ1-CH ₃ L62-δ2-CH ₃	T9- 5-CH ₃	Κ60-Ηα	
K60-Hδ2 K60-Hε1 K60-Hε2 L62-Hα L62-Hβ1 L62-Hβ2 L62- δ1-CH ₃ L62- δ2-CH ₃		К60-Нδ1	
K60-Hε1 K60-Hε2 L62-Hα L62-Hβ1 L62-Hβ2 L62- δ1-CH ₃ L62- δ2-CH ₃		К60-Нδ2	
K60-Hε2 L62-Hα L62-Hβ1 L62-Hβ2 L62- δ1-CH ₃ L62- δ2-CH ₃		K60-Hɛ1	
L62-Hα L62-Hβ1 L62-Hβ2 L62- δ1-CH ₃ L62- δ2-CH ₃		К60-Нε2	
L62-Hβ1 L62-Hβ2 L62- δ1-CH ₃ L62- δ2-CH ₃		L62-Ha	
L62-Hβ2 L62- δ1-CH ₃ L62- δ2-CH ₃		L62-Hβ1	
L62- δ1-CH ₃ L62- δ2-CH ₃		L62-Hβ2	
L62- 82-CH3		L62- δ1-CH ₃	
		L62- δ2-CH ₃	
Т10-Н6 L62- δ2-СН ₃	Т10-Н6	L62-δ2-CH ₃	
T10- 5-CH ₃ L62-Hβ1	T10- 5-CH ₃	L62-Hβ1	
L62-Нβ2		L62-Hβ2	
L62- δ1-CH ₃		L62- δ1-CH ₃	
L62- 82-CH ₃		L62- δ2-CH ₃	

	Table S3 Experimental restraints and structural statistics for A3A4M in complexes with
different ssDNA.	different ssDNA.

	A3A ^{NS} -DNA ^{NS}	A3A ^s -DNA ^s
Number of restraints		
Distance restraints from NOEs		
Total NOE	3346	3409
Intra-residue(i-j=0)	1613	1606
Sequential(i-j =1)	654	678
Medium range((1< i-j ≤5)	375	369
Long range(i-j >5)	654	661
Intermolecular (protein-DNA)	50	95
Inter-monomers		
Hydrogen bonds	170	174
Total dihedral angle restraints	369	369
Φ	184	184
Ψ	185	185
Structural statistics		
r.m.s.d versus the mean		
structure(Å)		
All backbone atoms	$1.57\pm0.23~\text{\AA}$	$1.46\pm0.46~\text{\AA}$
All heavy atoms	$1.91\pm0.19~\text{\AA}$	$1.79\pm0.38~\text{\AA}$
Backbone atoms (2 nd structure)	$0.55\pm0.11~\text{\AA}$	$0.54\pm0.07~\text{\AA}$
Heavy atoms (2 nd structure)	$1.13\pm0.09~\text{\AA}$	$1.16\pm0.13~\text{\AA}$
Rms Deviations from the		
experimental restraints		
NOE distance(Å)	0.035 ± 0.005	0.032 ± 0.001
Dihedral angels (deg)	1.37 ± 0.098	0.96 ± 0.11
Rms Deviations from idealized		
geometry		
Bonds(Å)	0.0025 ± 0.00017	0.0027 ± 0.00010
Angels(deg.)	0.38 ± 0.013	0.42 ± 0.029
Impropers(deg.)	0.31 ± 0.018	0.32 ± 0.013
Ramachandran Analysis		
residues in most favored	89.0%	86.6%
regions		
residues in additionally allowed	9.8%	11.7%
regions		
residues in generously allowed	1.2%	1.7%
regions		
residues in disallowed regions	0.0%	0%

Supplemental References

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