

Supporting Information:

Signatures of specific DNA binding by the AT-rich interaction domain of BAF250a

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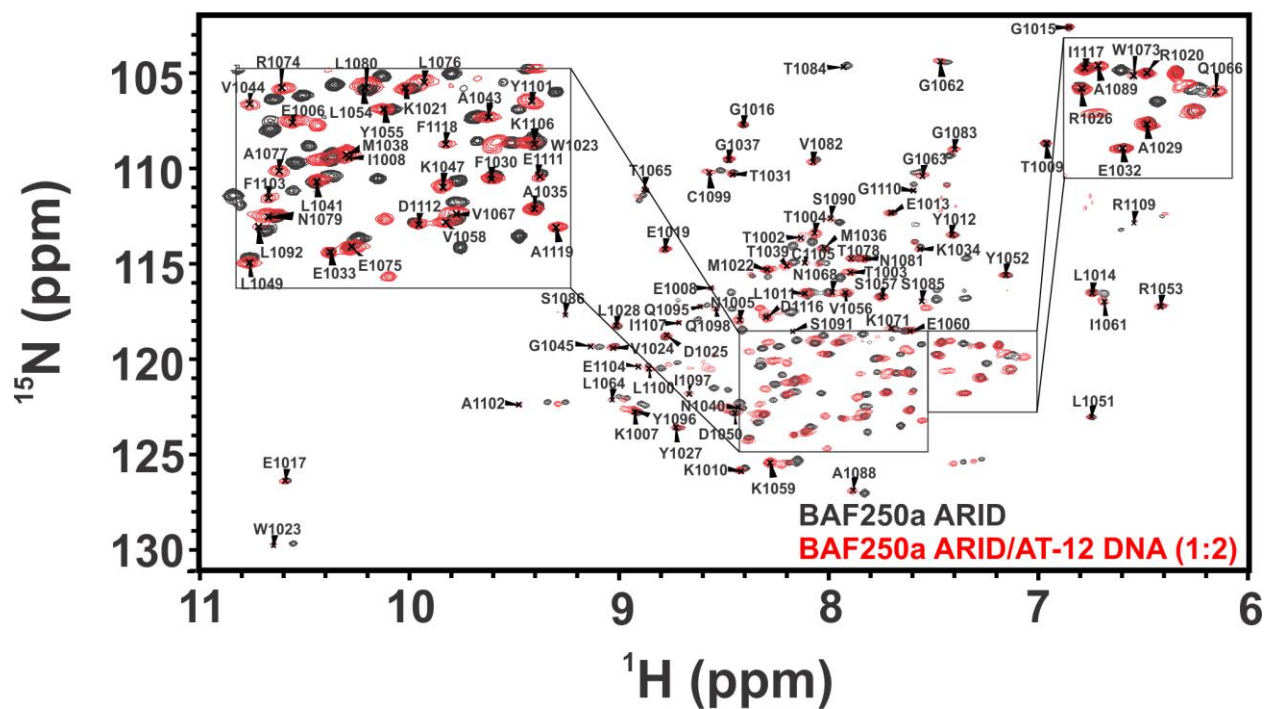


Figure S1. Overlay of 2D ^1H - ^{15}N TROSY-HSQC spectra of free BAF250a ARID (black) and BAF250a ARID/AT-12 DNA complex (red) with the assignment of the cross peaks marked in the spectra (taken from BMRB entry with accession code 5748).

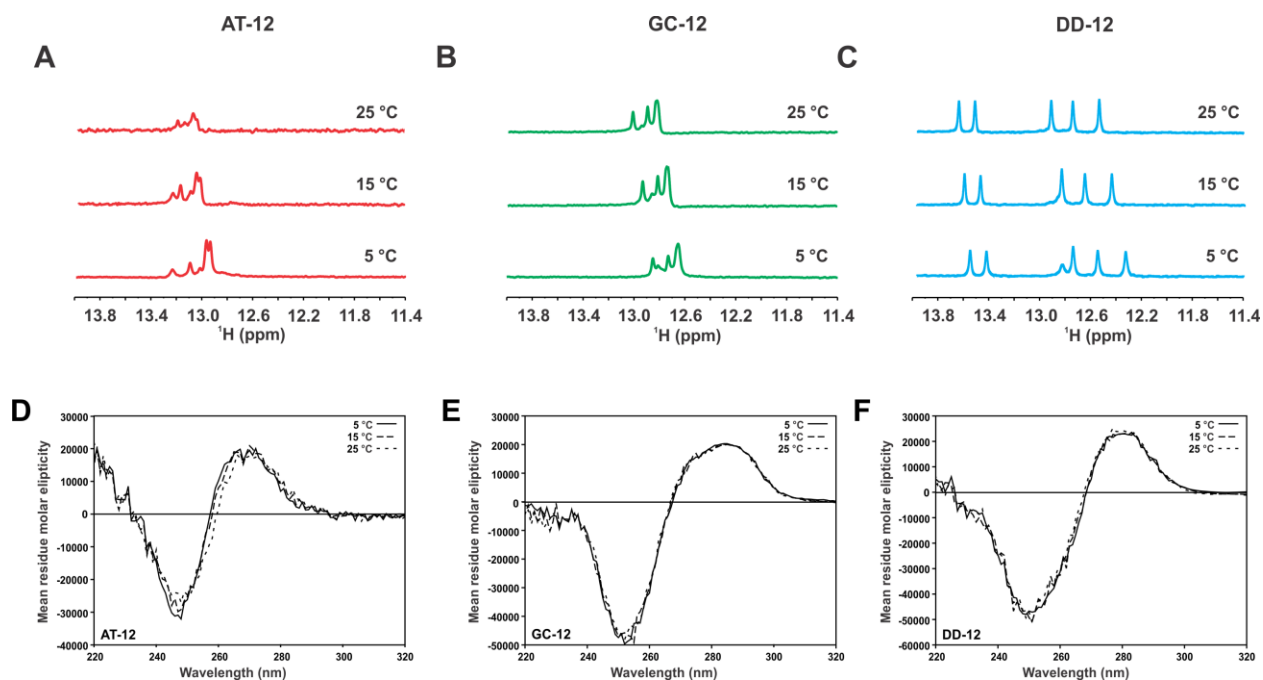


Figure S2. 1D ^1H NMR and CD spectra of dsDNA sequences used in this study at different temperatures. (A) 1D ^1H NMR spectra of AT-12 DNA. (B) 1D ^1H NMR spectra of GC-12 DNA. (C) 1D ^1H -NMR spectra of DD-12. (D-F) Overlay of CD spectra recorded at 5°C, 15°C and 25°C for (D) ds AT-12 (E) GC-12 and (F) DD-12 DNA.

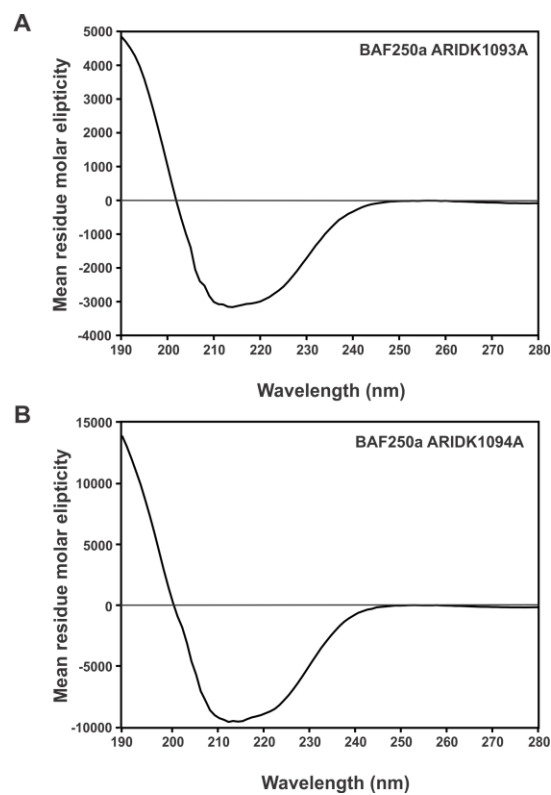


Figure S3. Analysis of BAF250a ARID mutants using CD spectroscopy. (A) CD spectrum of BAF250a ARID K1093A. (B) CD spectrum of BAF250a ARID K1094A.

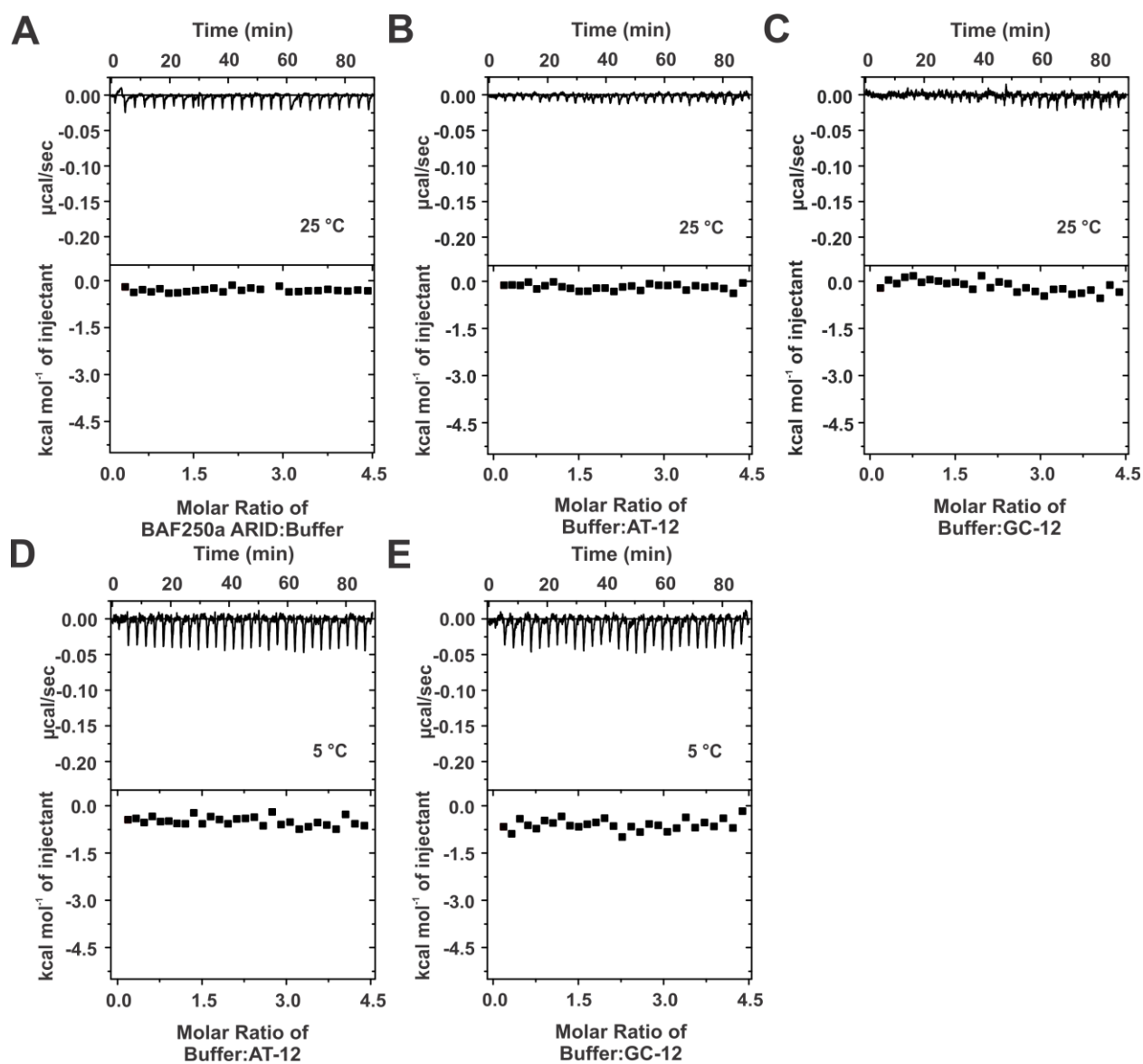


Figure S4. ITC isotherms for the 'control' protein into buffer and buffer into DNA titrations. (A) Heat of dilution of BAF250a ARID titrated into buffer at 25 °C. (B) Heat of dilution of buffer titrated into AT-12 DNA at 25 °C. (C) Heat of dilution of buffer titrated into GC-12 DNA at 25 °C. (D) Heat of dilution of buffer titrated into AT-12 DNA at 5 °C. (E) Heat of dilution of buffer titrated into GC-12 DNA at 5 °C.

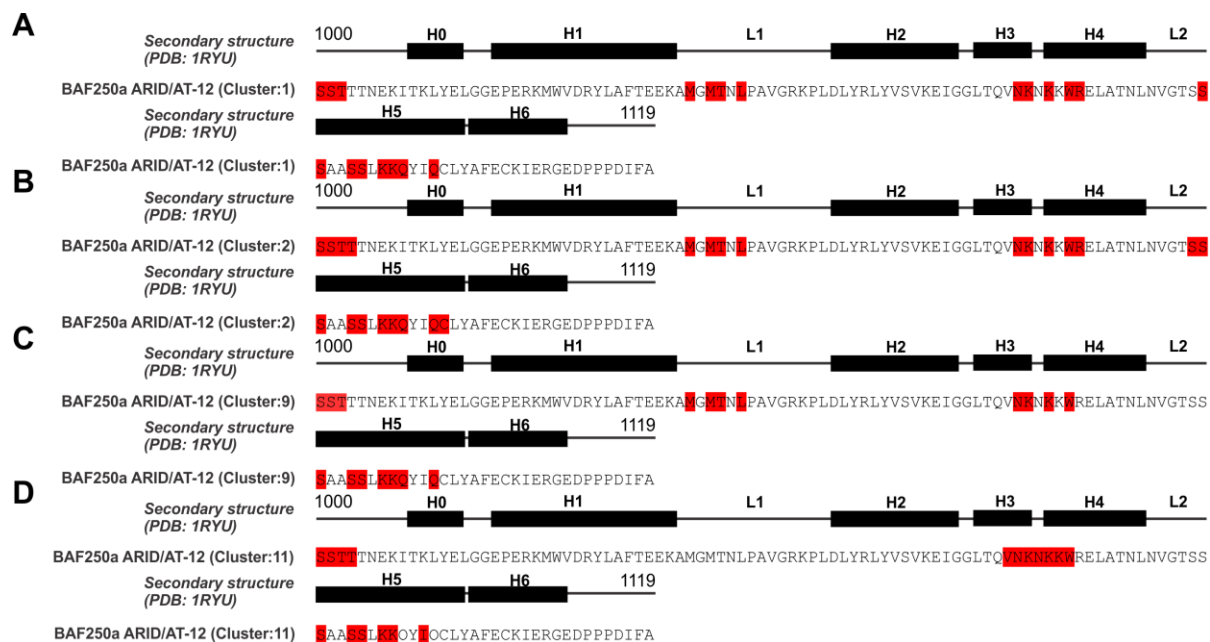


Figure S5. Plausible mode of DNA binding by BAF250a ARID in the four major clusters of HADDOCK models. (A-D) The DNA binding residues in top structures from four clusters are marked on the secondary structures of BAF250a ARID. The four clusters are: (A) Cluster 1 (B) Cluster 2 (C) Cluster 9 and (D) Cluster 11. The sequence and secondary structure of BAF250a ARID are shown. The helices are shown in black rectangle. The residues that contact AT-12 DNA in HADDOCK model structures are highlighted in red.

TABLE S1. Statistics for the NMR CSP driven HADDOCK model of BAF250a ARID in complex with AT-12 DNA

Parameter	Value
HADDOCK score	-107.6 \pm 2.5 a.u.
Cluster size	29
RMSD from the overall lowest-energy structure	13.5 \pm 0.2 Å ²
Van der Waals energy	-64.9 \pm 10.0 kcal mol ⁻¹
Electrostatic energy	-374.6 \pm 31.8 kcal mol ⁻¹
Desolvation energy	10.5 \pm 6.6 kcal mol ⁻¹
Restraints violation energy	216.9 \pm 50.98 kcal mol ⁻¹
Buried surface area	1863.7 \pm 146.7 Å ²
Z-score	-0.5