Supplemental Data

Solution structure and molecular interactions of the Lamin B Receptor Tudor domain

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Supplementary Table 1. Structural statistics for the TUDOR domain of LBR

NOE and hydrogen bond distance restraints		
Total	825	
Intraresidue	215	
Sequential	212	
Medium range (1<i<5)	80	
Long range (i>5)	318	
Hydrogen bond restraints	44	
Dihedral angle restraints (φ and ψ)	68	
CYANA target function value (Å^2)	0.91±0.03 [a]	1.91±0.51 [b]
Restraint violations		
Distance restraint violations (>0.2Å)	2 [a]	0 [b]
Dihedral angle restraint violations (>5.0°)	2 [a]	0 [b]
RMSD deviation from the average coordinates (Å)		
Backbone atoms (residues 8-62)	0.32±0.11[a]	0.53±0.11[b]
Heavy atoms	0.82±0.07 [a]	1.03±0.09 [b]
WHATIF quality check		
Packing	-2.24[a]	-1.31[b]
Ramachandran	-2.89 [a]	-2.68 [b]
PROCHECK ramachandran plot analysis (%)		
Residues in most favored regions	78.9[a]	91.2[b]
Residues in additional allowed regions	17.5 [a]	7.0 [b]
Residues in generously allowed regions	3.5 [a]	1.8 [b]
Residues in disallowed regions	0.0 [a]	0.0 [b]

[a]before water refinement
[b]after water refinement

Supplementary Figure S1

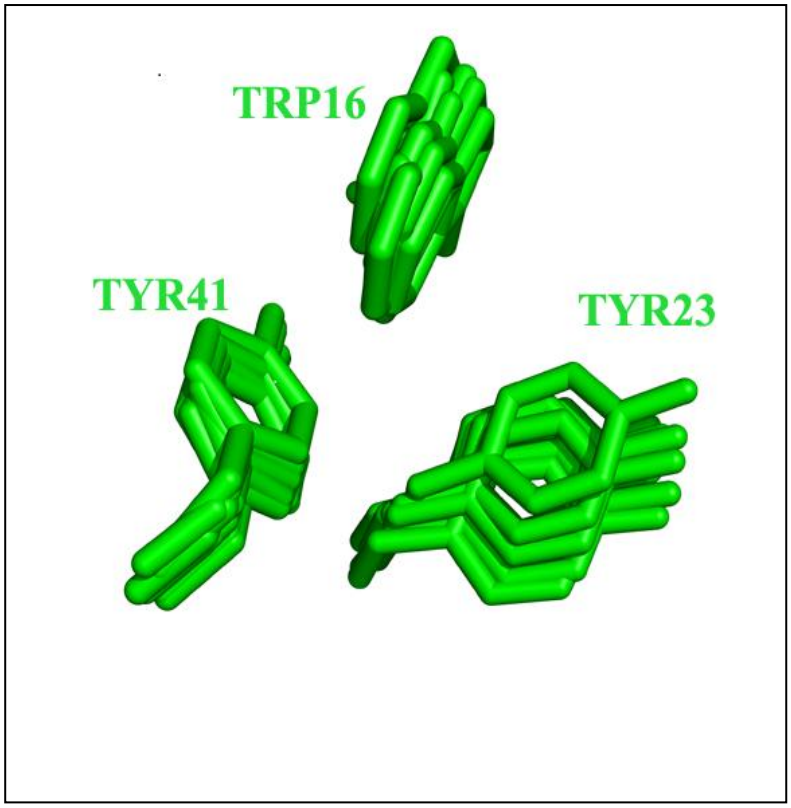

Fig. S1: Superposition of the aromatic cluster of LBR-TD in the ensemble of the 10 lowest energy structures. The number of NOE restrains originating from the aromatic residues are: 54 (for Trp16), 38 (for Tyr23) and 60 (for Tyr41).

Supplementary Figure S2

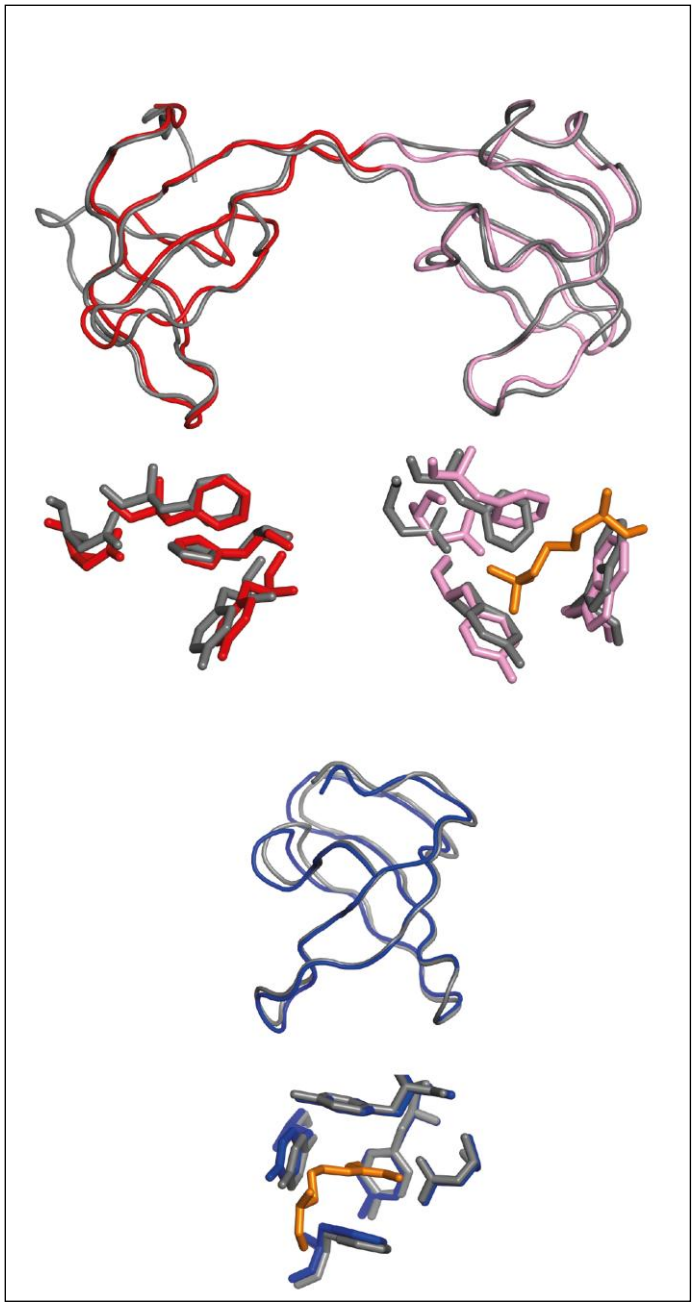

Fig. S2: Superposition of free and bound forms for the interdigitated Tudor domains of JMJD2A (top) and the Tudor domain of SND1 (bottom). Each panel depicts the overall fold in cartoon-loop representation and the aromatic cage residues in stick representation. Free forms are shown in gray and the bound ones in color. The corresponding methylated ligands are shown as sticks and colored orange. PDB codes as in Figure 2.

Supplementary Figure S3

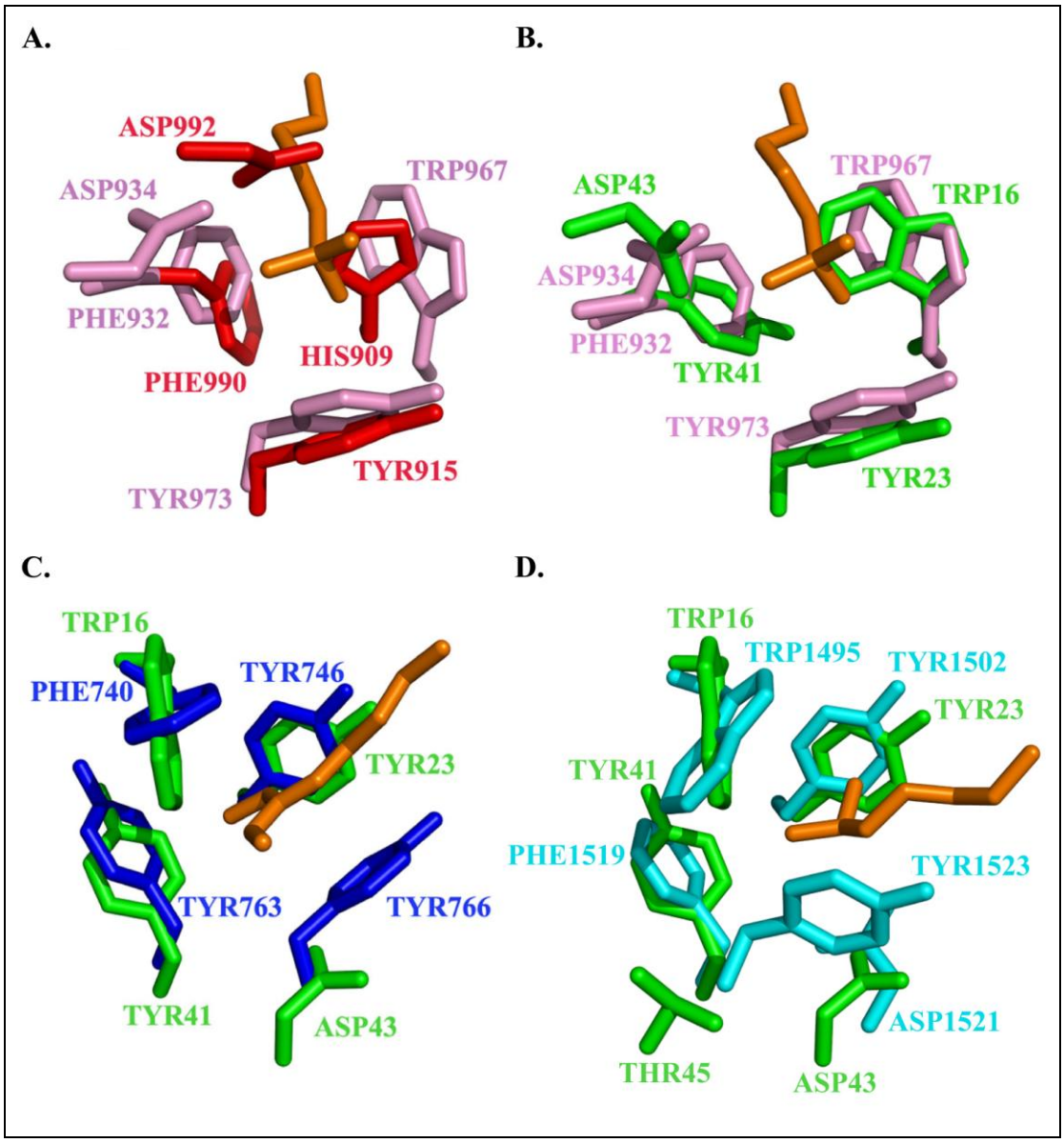

Fig. S3: Comparison of the aromatic cage of LBR-TD with those of SND1 and JMJD2A. A. Superimposition of the two aromatic clusters of HTD1 (pink) and HTD2 (red) from JMJ2DA. B. Superimposition of the aromatic clusters of LBR-TD (green) with the one from JMJ2DA-HTD2 (magenta) complexed with H3K4me3 (orange) [15]. C. Superimposition of the aromatic clusters of LBR-TD (green) with the one from SND1(blue) complexed with a symmetrically dimethylated Arg peptide (orange) derived from the Piwi protein PIWIL1 [12]. D. Superimposition of the aromatic clusters of LBR-TD (green) with the one from 53BP1 (cyan) complexed with H4-K20me2 (orange) [14]. PDB codes as in Figure 2.

Supplementary Figure S4

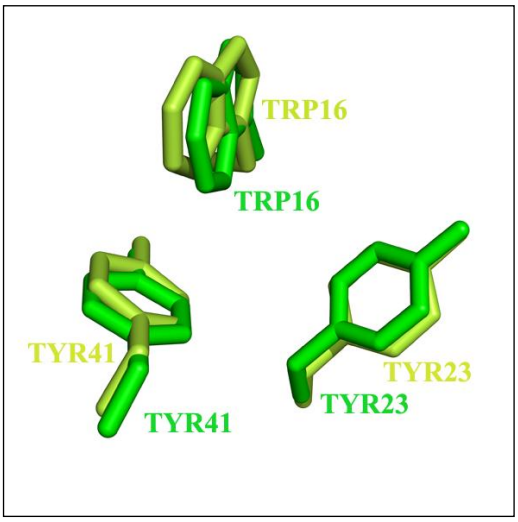

Fig. S4: Superimposition of the aromatic clusters of LBR-TD from human (2dig) in yellow and from chicken (in green).

Supplementary Figure S5

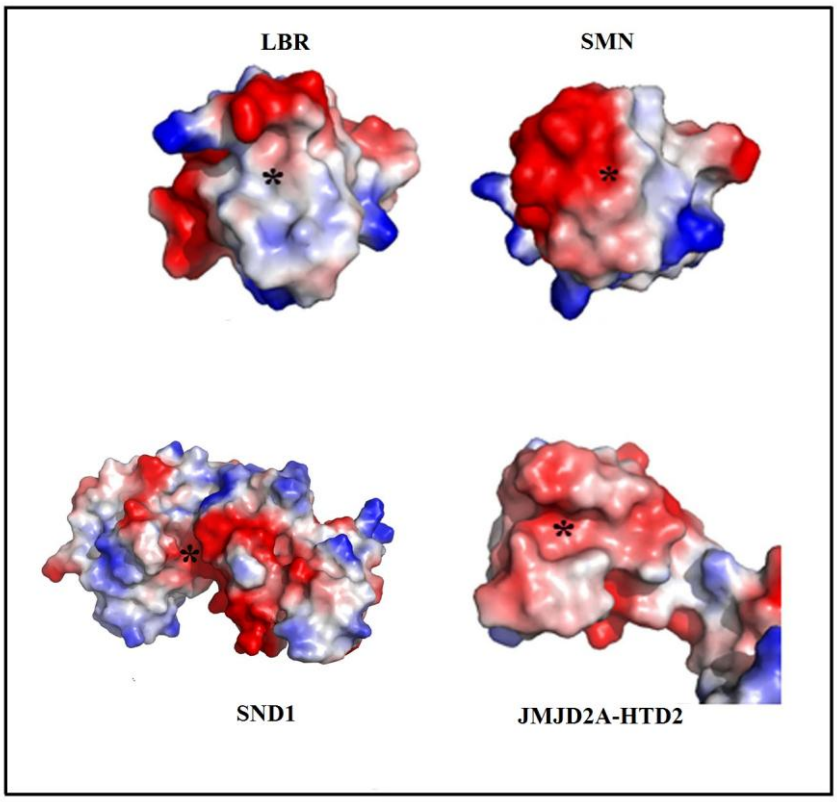

Fig. S5: Comparison of surface characteristics of homologous Tudor domains. Electrostatic surface representation of LBR-TD, SMN-TD, SND1-TD and JMJ2DA- HTD2 domains. Red and blue indicates negative and positive charge respectively. The star symbol (*) indicates the position of the aromatic cage. PDB codes as in Figure 2.