

# Supplementary Information

## Comparison of Empirical $\text{Zn}^{2+}$ Models in Protein-DNA Complexes

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Table S1: Protonation states of cysteines and histidines in MLL1 and WT1.

<b>System</b>	<b>Residue</b>	<b>Index</b>	<b><math>\text{Zn}^{2+}</math> (residue)</b>
MLL1	CYM1167	17	ZN1 (ZN1301)
	CYM1170	20	
	CYM1173	23	
	CYM1189	39	
MLL1	CYM1155	5	ZN2 (ZN1302)
	CYM1158	8	
	CYM1161	11	
	CYM1194	44	
WT1	CYM355	5	ZN1 (ZN505)
	CYM360	10	
	HID373	23	
	HID377	27	
WT1	CYM385	35	ZN2 (ZN506)
	CYM388	38	
	HID401	51	
	HID405	55	
WT1	CYM413	63	ZN3 (ZN507)
	CYM418	68	
	HID431	81	
	HID435	85	
WT1	HIE397	47	—
	HID432	82	—

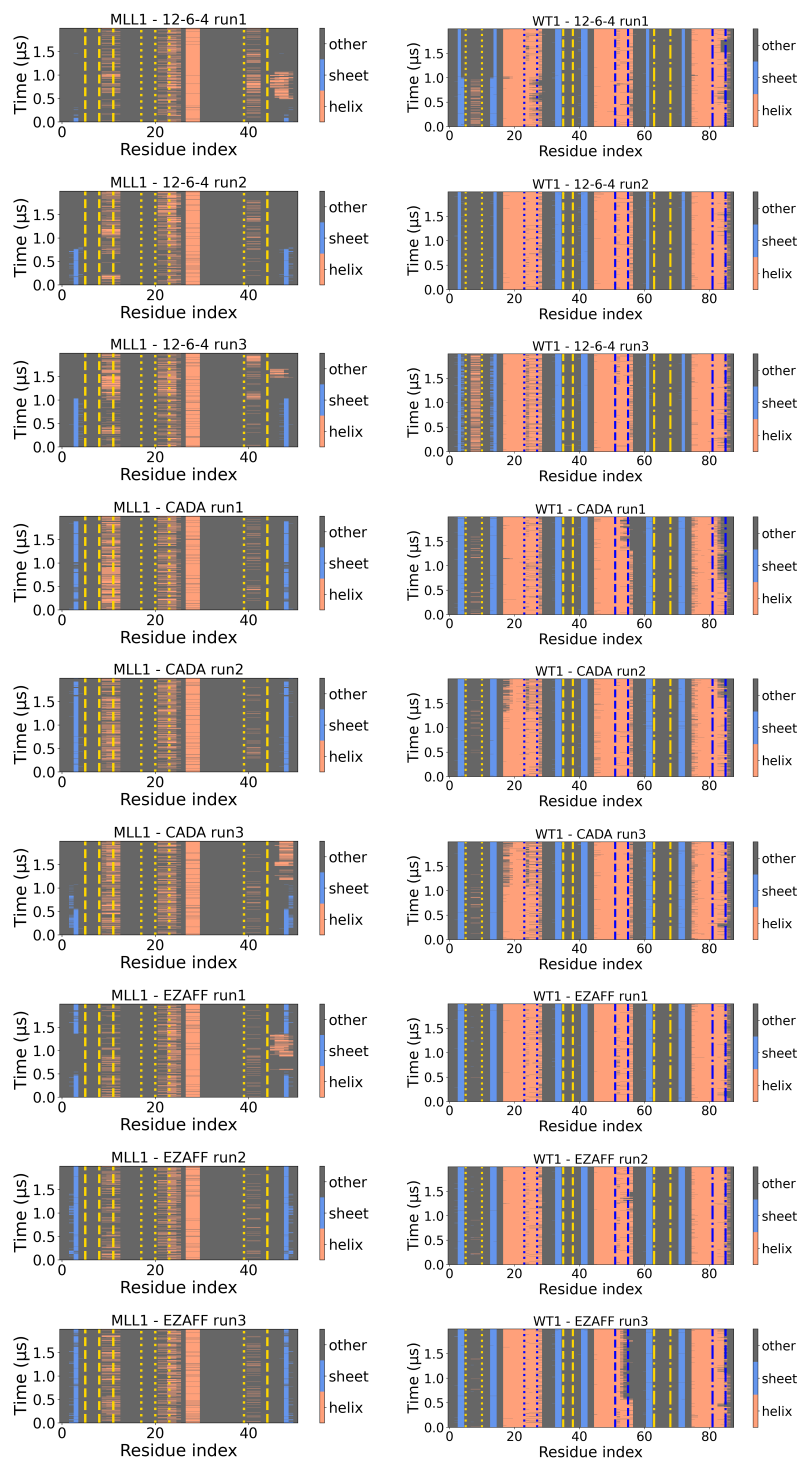


Figure S1: Secondary structure elements for all protein residues over the course of simulation for WT1 and MLL1; helices are shown in light red, sheets in light blue and everything else in grey colour. Coordinating cysteines are shown in yellow and histidines in blue. The residues coordinating ZN1, ZN2 and ZN3 are indicated as dotted, dashed and dash-dotted lines, respectively.

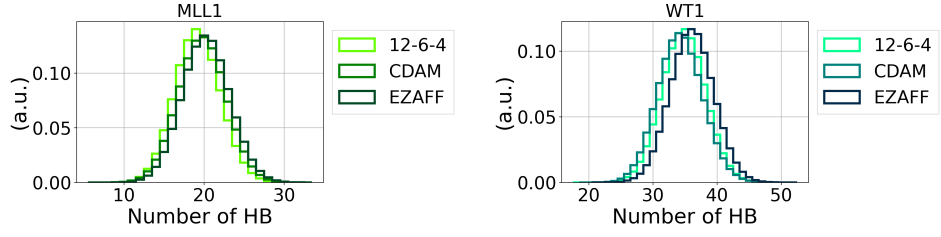


Figure S2: Number of hydrogen bonds within protein for MLL1 (left) and WT1 (right).

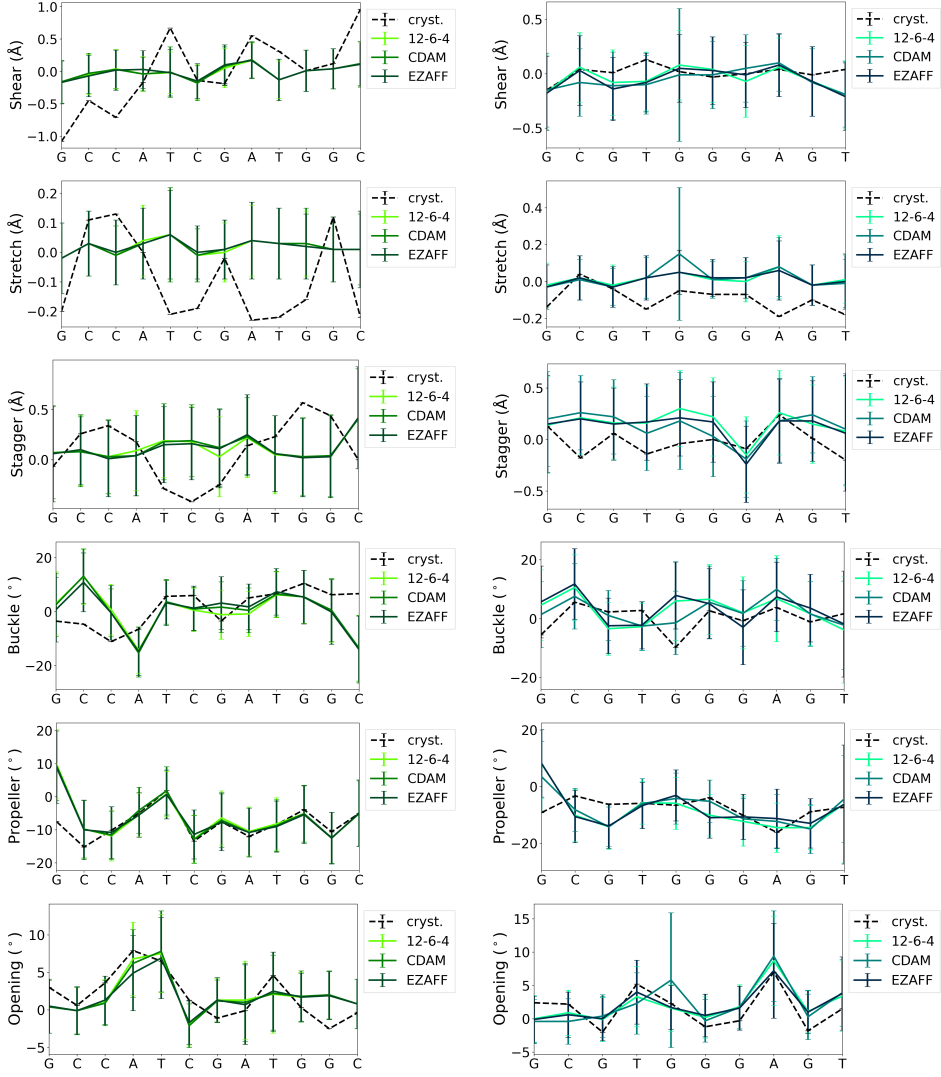


Figure S3: DNA intra-base pair parameters for MLL1 (left) and WT1 (right).

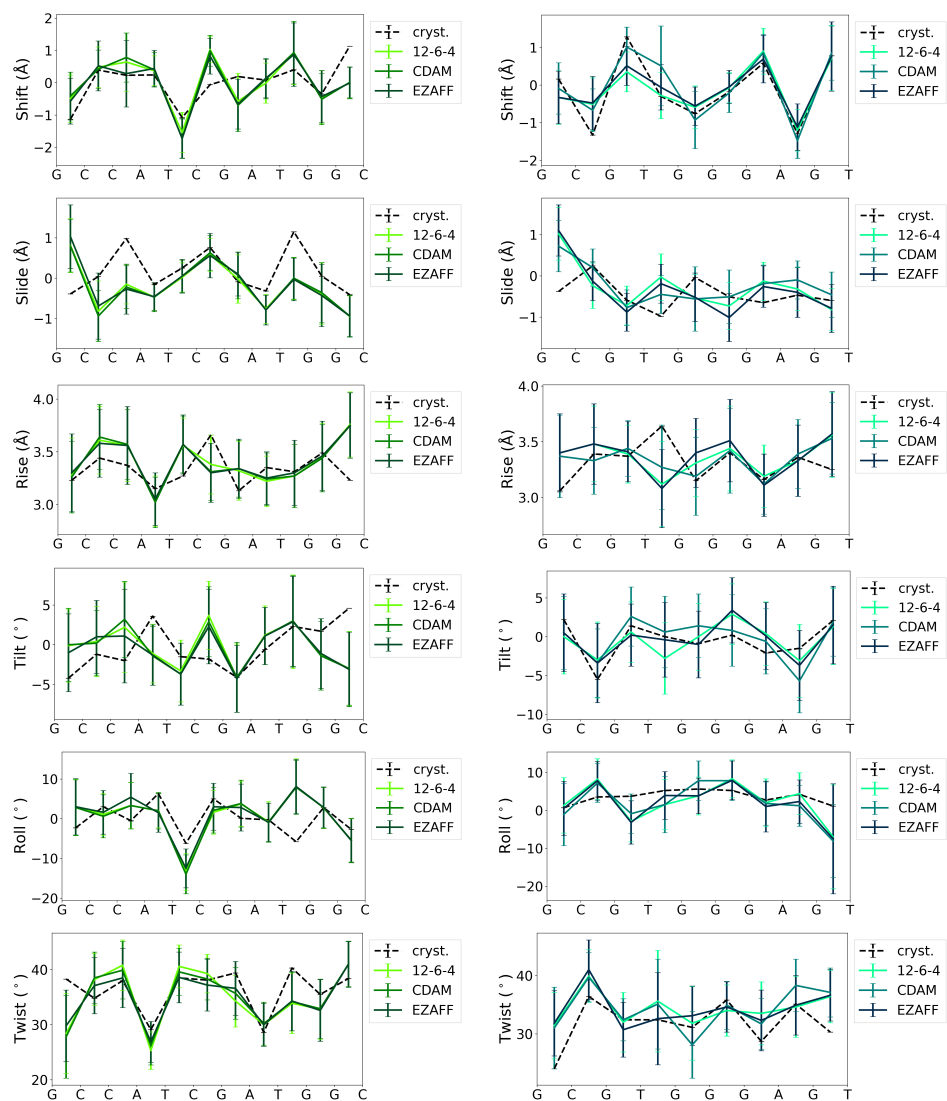


Figure S4: DNA inter-base pair parameters for MLL1 (left) and WT1 (right).



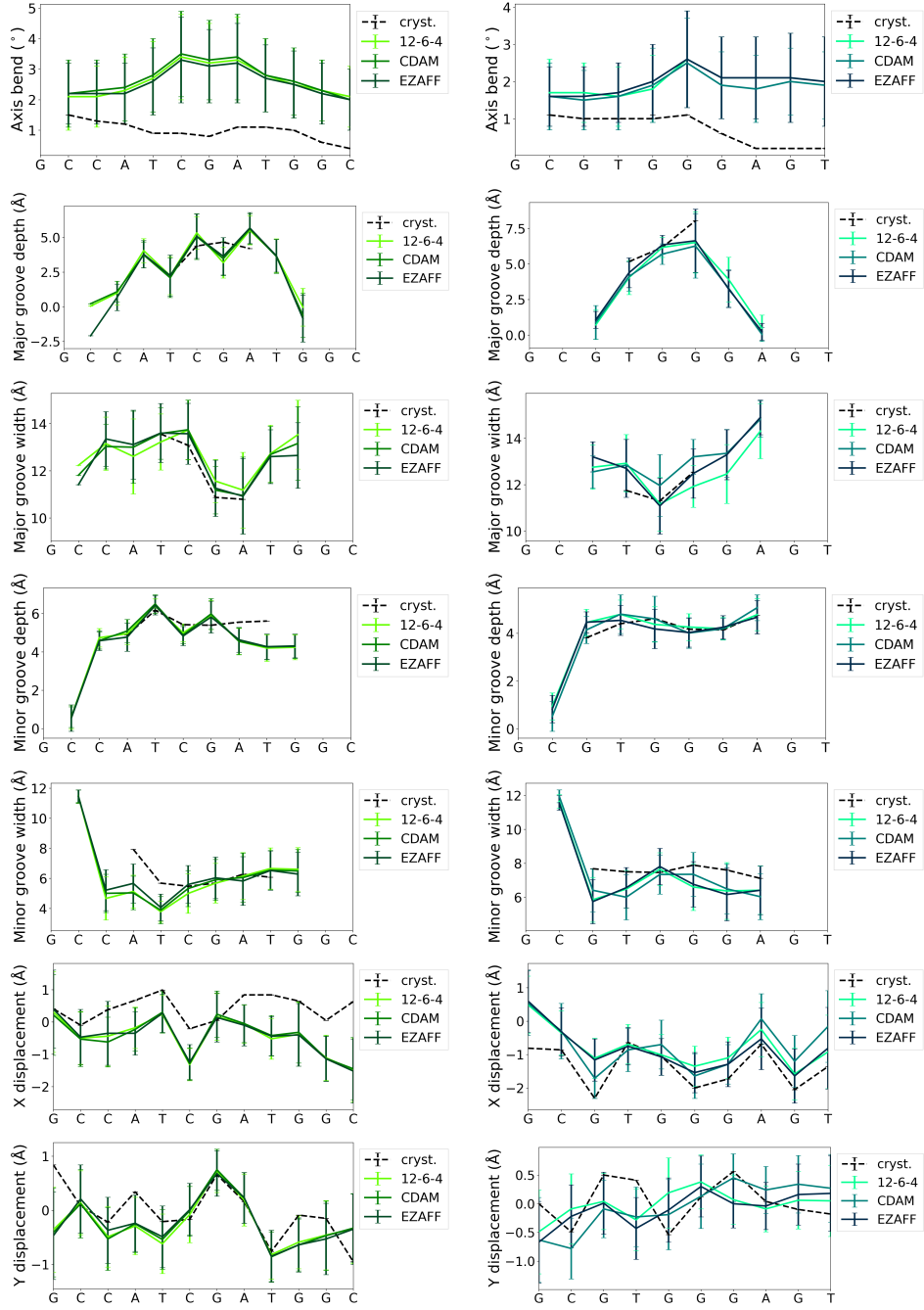


Figure S5: DNA axis parameters for MLL1 (left) and WT1 (right).

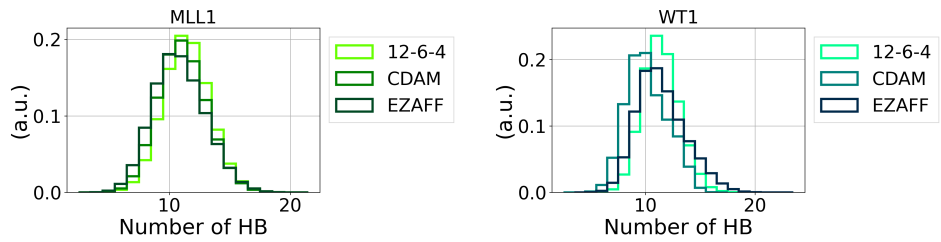


Figure S6: Number of hydrogen bonds between protein and DNA for MLL1 (left) and WT1 (right).

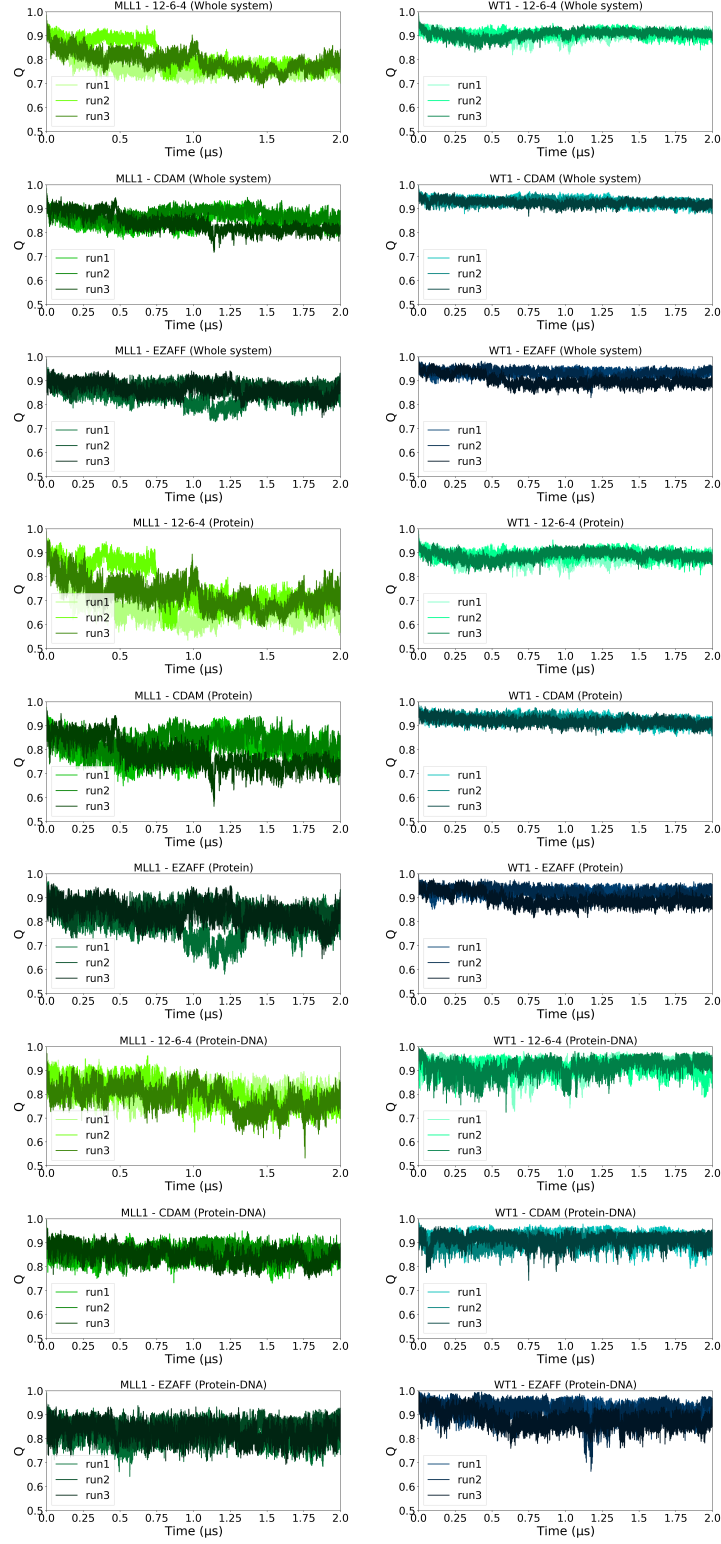


Figure S7: Fraction of native contacts time series of the whole system, within protein and between protein and DNA for MLL1 (left) and WT1 (right).

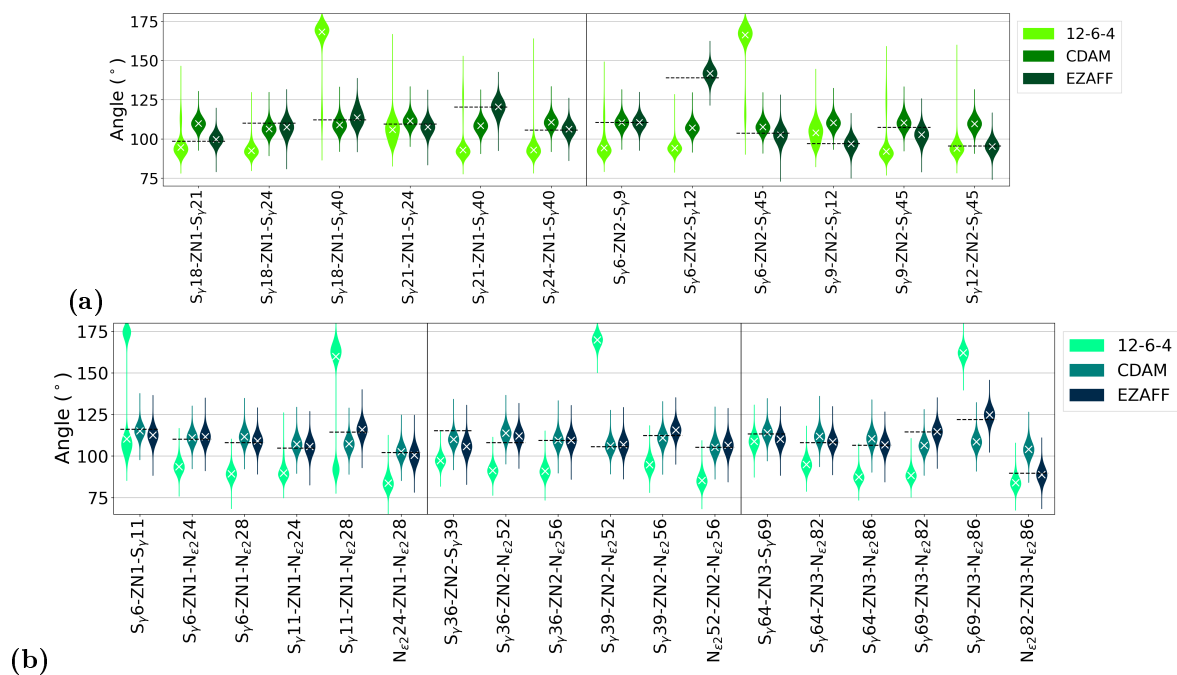


Figure S8: Angles around the  $\text{Zn}^{2+}$ -ions including their coordinating ligands for (a) MLL1 and (b) WT1. The median values are shown as white x. Crystal structure values are indicated as black dashed lines.

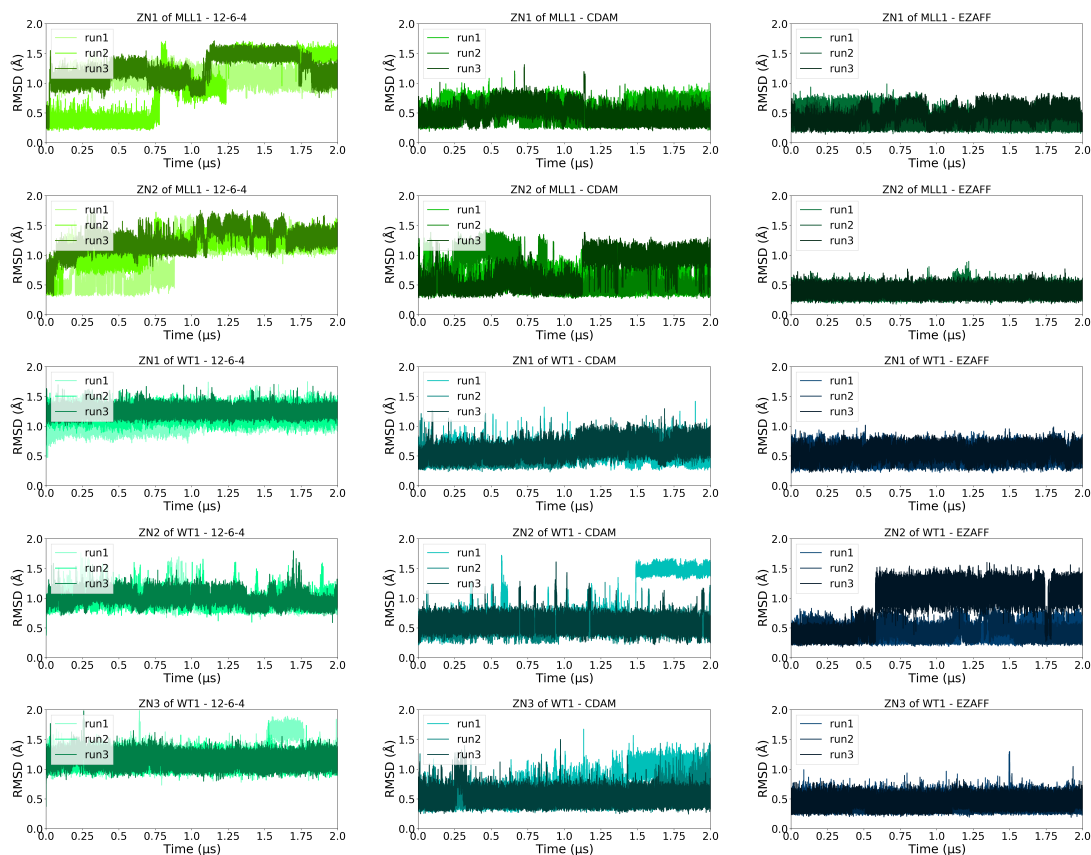


Figure S9: RMSD of  $\text{Zn}^{2+}$ -ions and their ligating residues of MLL1 and WT1 in all three ion models with respect to the crystal structure.

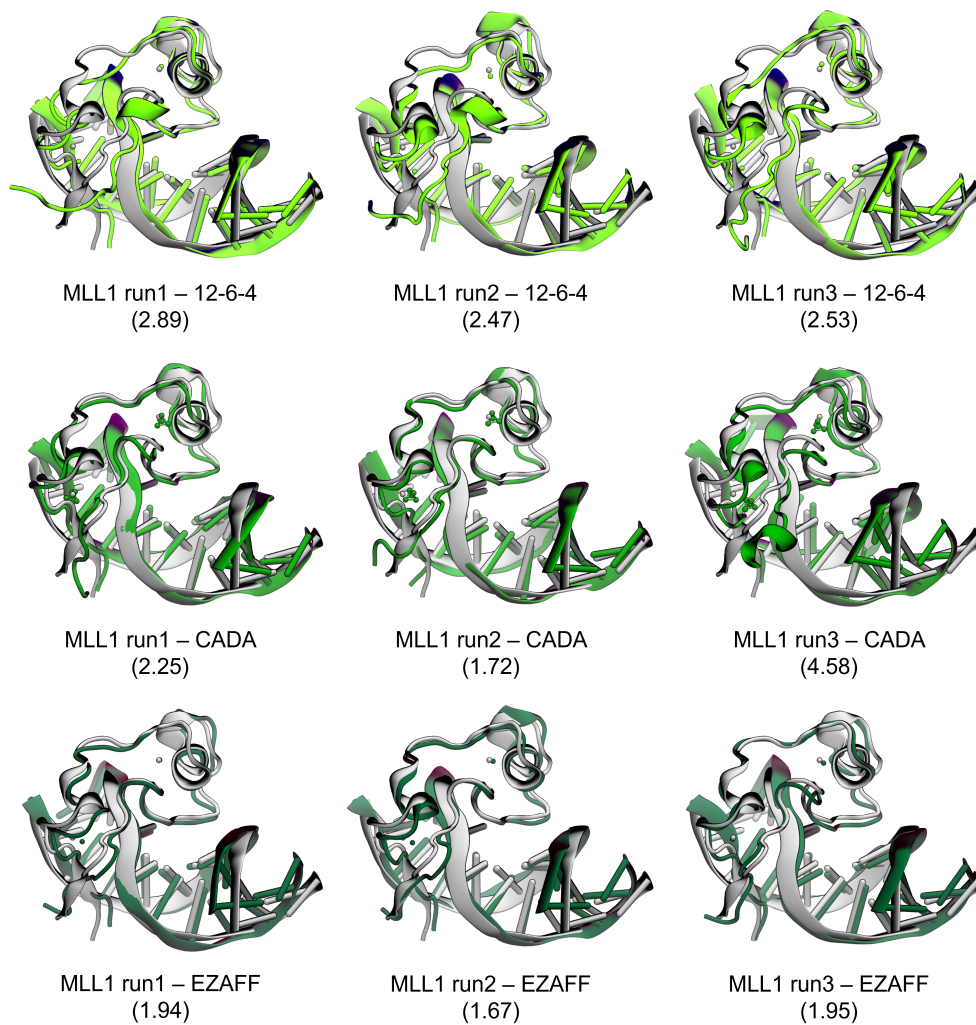


Figure S10: Median structures of the last 100 ns of all simulation runs of MLL1 aligned (protein and DNA backbone) to the corresponding crystal structure (grey). RMSD values in Å of protein and DNA backbone with respect to the crystal structure are shown in parentheses.

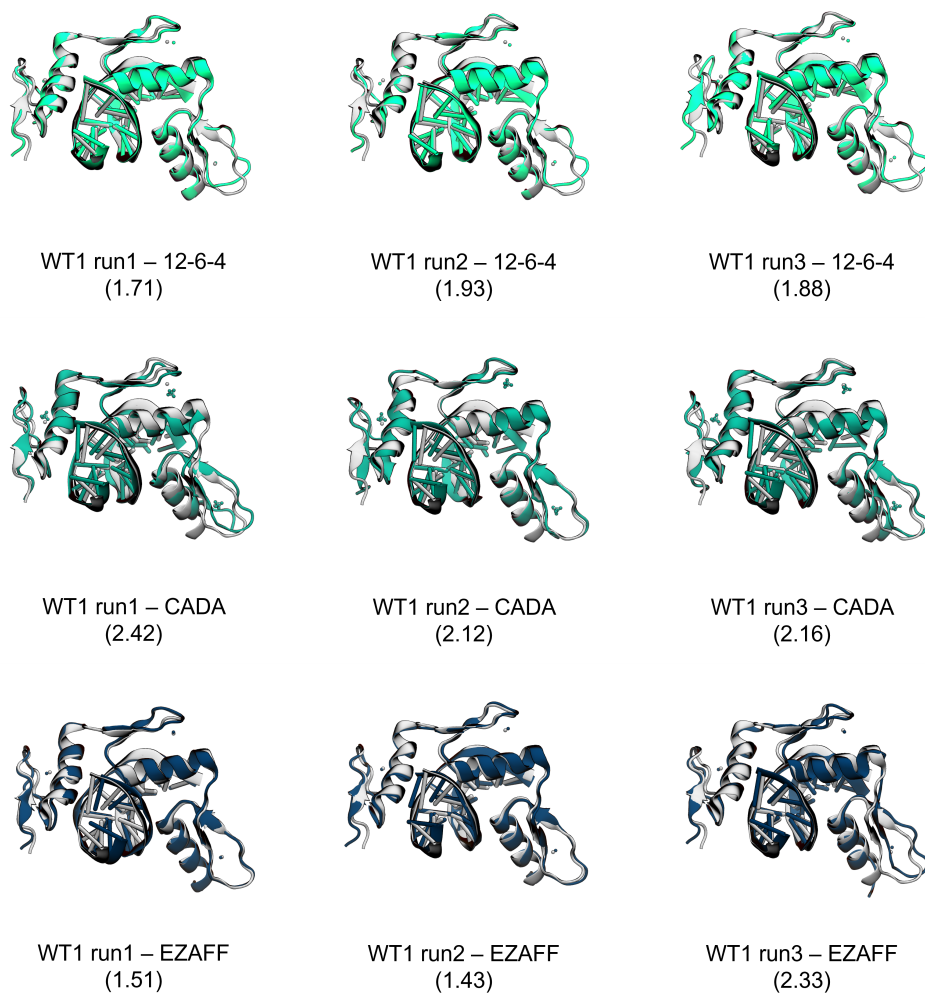


Figure S11: Median structures of the last 100 ns of all simulation runs of WT1 aligned (protein and DNA backbone) to the corresponding crystal structure (grey). RMSD values in Å of protein and DNA backbone with respect to the crystal structure are shown in parentheses.