Molecular Dynamics Simulations of Protein RNA Complexes by Using an Advanced Electrostatic Model

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Simulations of RNA and DNA systems

The optimized parameters were tested on several RNA and DNA systems following the procedure in our previous work.[1] Three 1000-ns simulations were performed for tetranucleotides AAAA and GACC. Two 500-ns simulations were performed for 2JXQ, 2KOC and 1NAJ. The AAAA simulations had slightly lower percentage of A-form conformation compared to the simulations with the original AMOEBA parameters, while the GACC system had slightly higher percentage of A-form. Simulations of an RNA duplex, an RNA hairpin and a DNA duplex resulted in slightly higher RMSDs to the crystal structure than simulations with the original parameters.

Table S1. Numbers of model dimer structures for protein-nucleic acid interactions with PDB geometry

	A	T	U	G	C
A	15				
T	14	10			
U	29	2	15		
G	35	19	34	25	
C	25	15	25	21	16
NMA	19	17	17	16	19
EtOH	7	8	9	9	9
Acetate	10	12	11	11	12
MeNH3	6	4	4	5	4
Imidazole	14	12	12	14	12
Benzene	16	17	17	18	16

Table S2. Root mean squared deviations (Å) of DNA and RNA systems in AMOEBA simulations.

		RMSD(amoebabio18)		RMSD(this work)	
Type	PDB	Non-terminal	Heavy-atom	Non-terminal	Heavy-atom
RNA duplex	2JXQ	1.25	1.98	1.588	2.598
		1.41	2.38	1.416	2.385
RNA hairpin	2KOC	1.72	1.78	1.93	1.983
		1.9	1.95	1.901	1.977
B-DNA duplex	1NAJ	1.29	2.54	1.439	2.17
				1.532	2.343

For each system, the results of two independent simulations are listed.

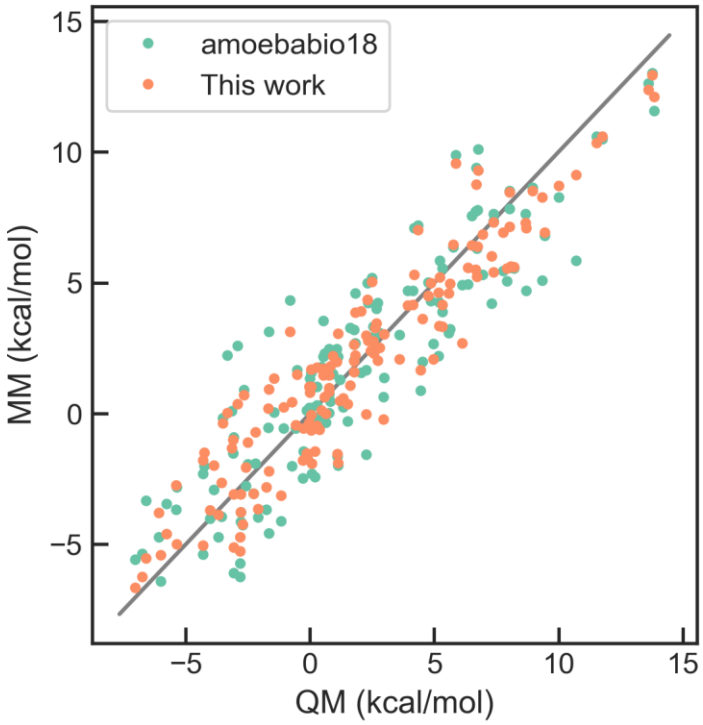

Figure S1. Correlation between QM and MM relative energies for the Asn conformers generated from one-dimensional torsion scan and rotamer library.

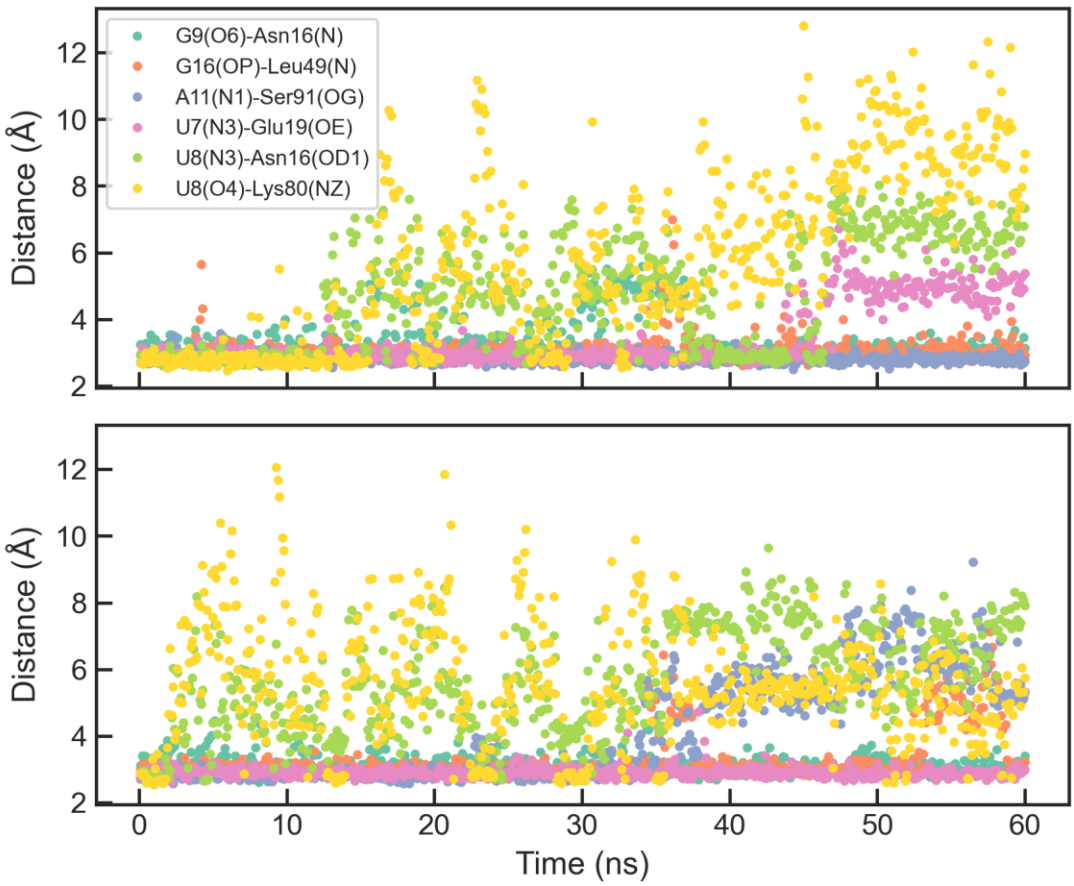

Figure S2. Evolution of selected hydrogen-bond distances in simulations of U1A with optimized vdW parameters.

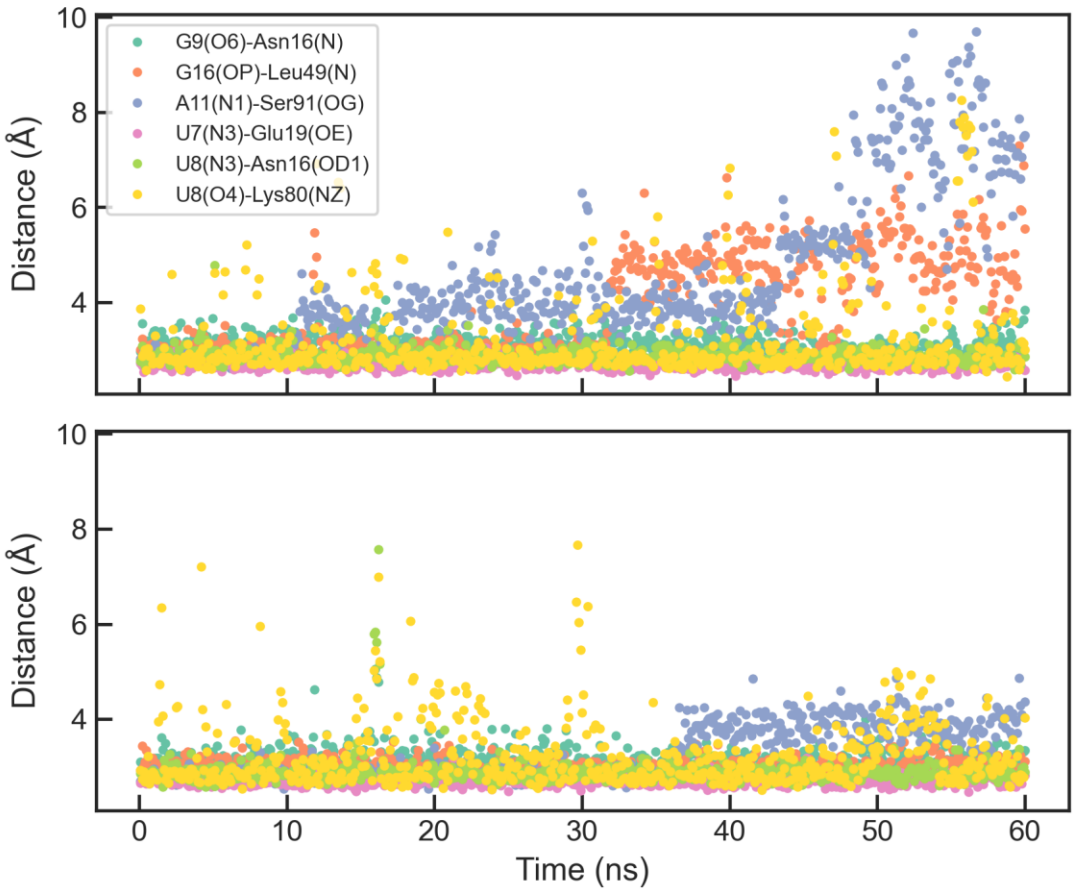

Figure S3. Evolution of selected hydrogen-bond distances in simulations of U1A with optimized vdW and Asn side-chain torsion parameters.

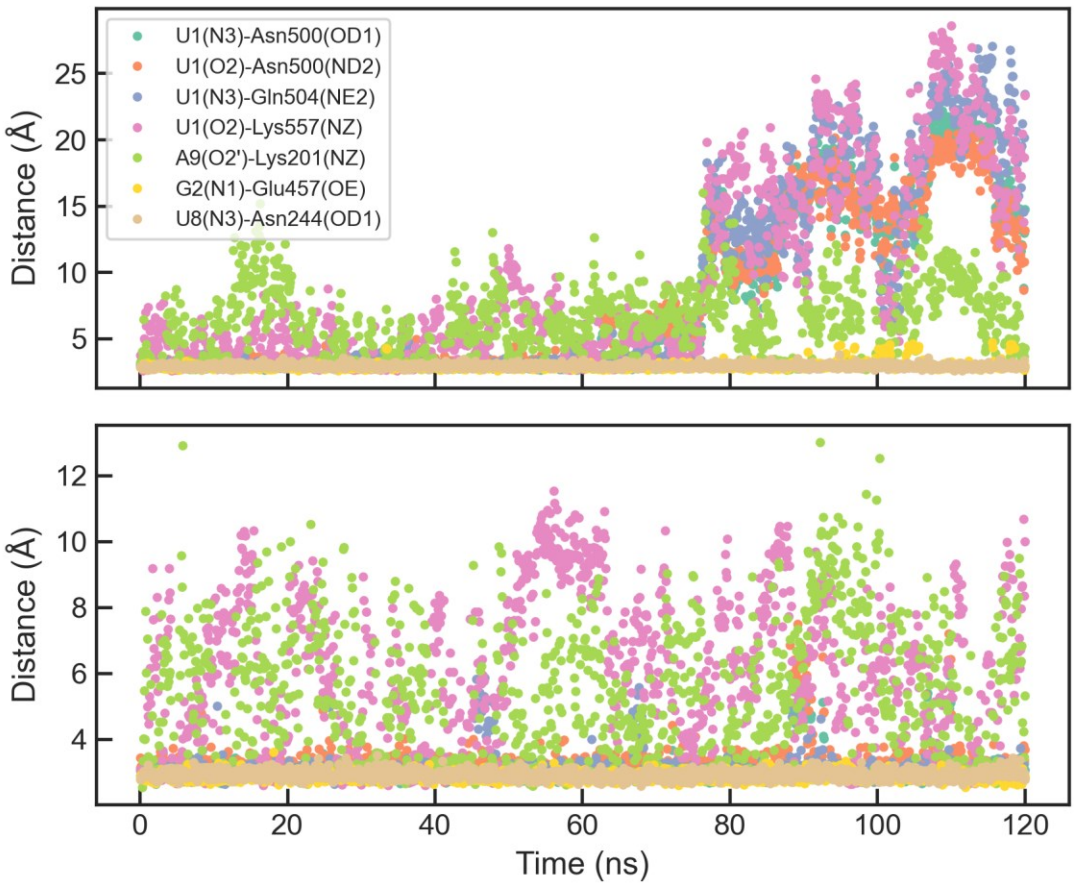

Figure S4. Evolution of selected hydrogen-bond distances in simulations of FBF with original AMOEBA parameters.

References

(1) Zhang, C.; Lu, C.; Jing, Z.; Wu, C.; Piquemal, J.-P.; Ponder, J. W.; Ren, P. AMOEBA Polarizable Atomic Multipole Force Field for Nucleic Acids. *J. Chem. Theory Comput.* **2018**, *14* (4), 2084-2108. DOI: 10.1021/acs.jctc.7b01169.