CONFORMATIONAL HETEROGENEITY OF UCAAUC RNA OLIGONUCLOTIDE FROM MOLECULAR DYNAMICS SIMULATIONS, SAXS, AND NMR EXPERIMENTS

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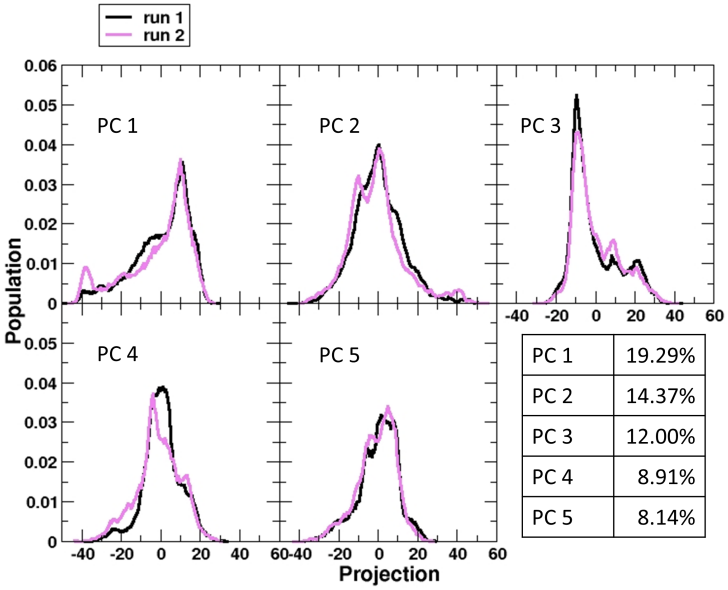
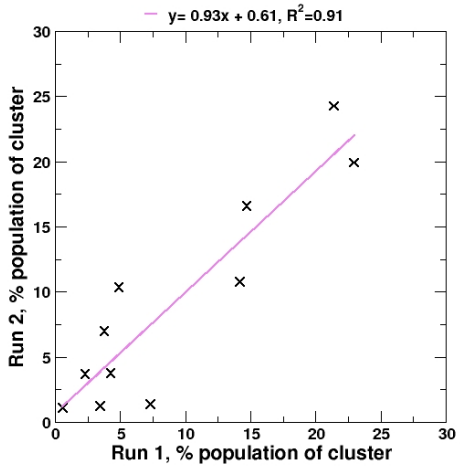
SUPPORTING INFORMATION

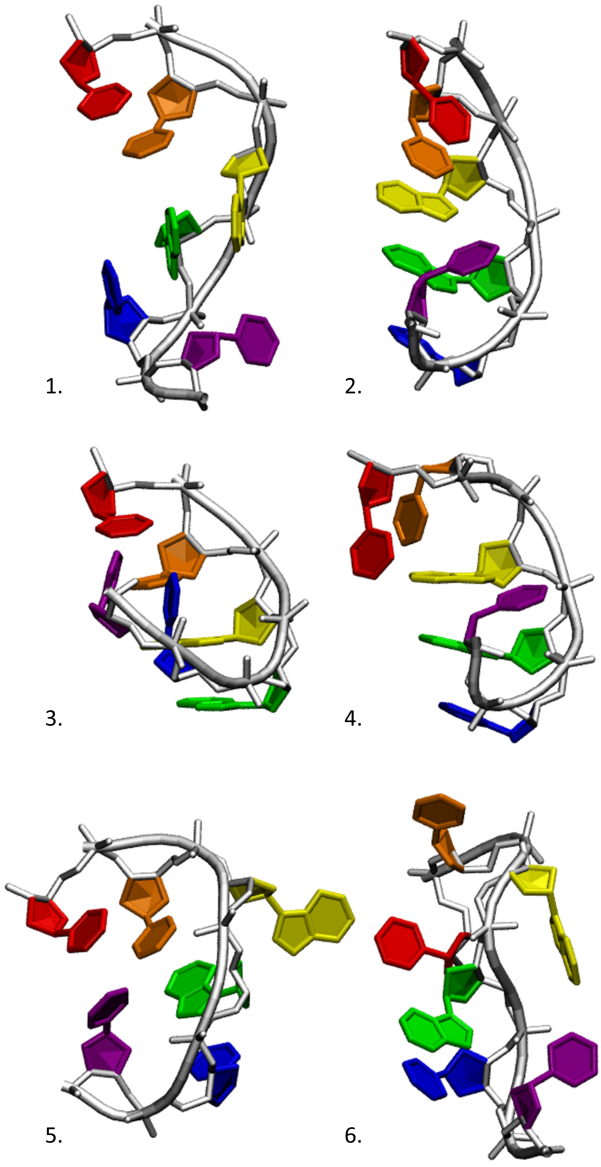


PC 1	19.29%
PC 2	14.37%
PC 3	12.00%
PC 4	8.91%
PC 5	8.14%

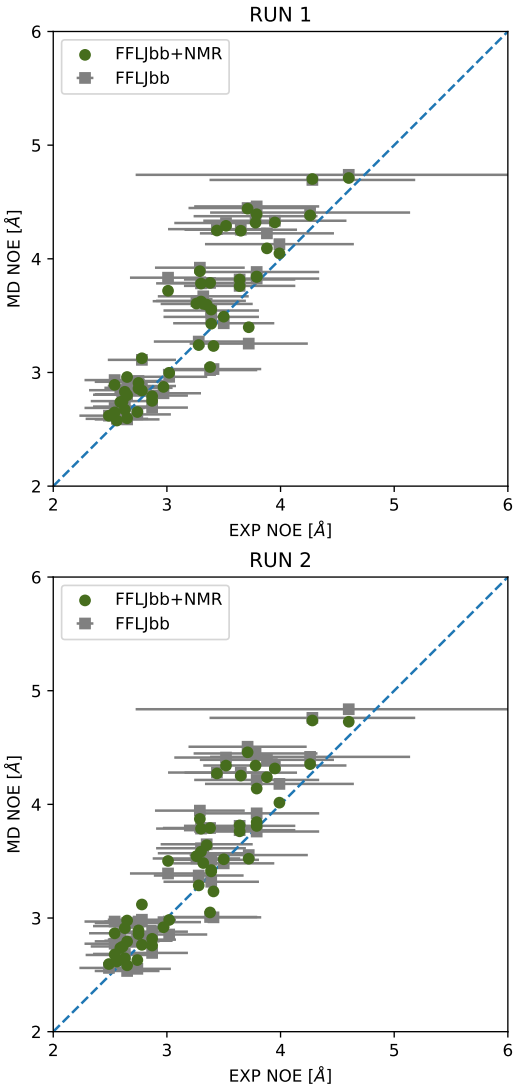
SI1: Principal component analysis of two independent MD simulations using the FFLJbb force field.



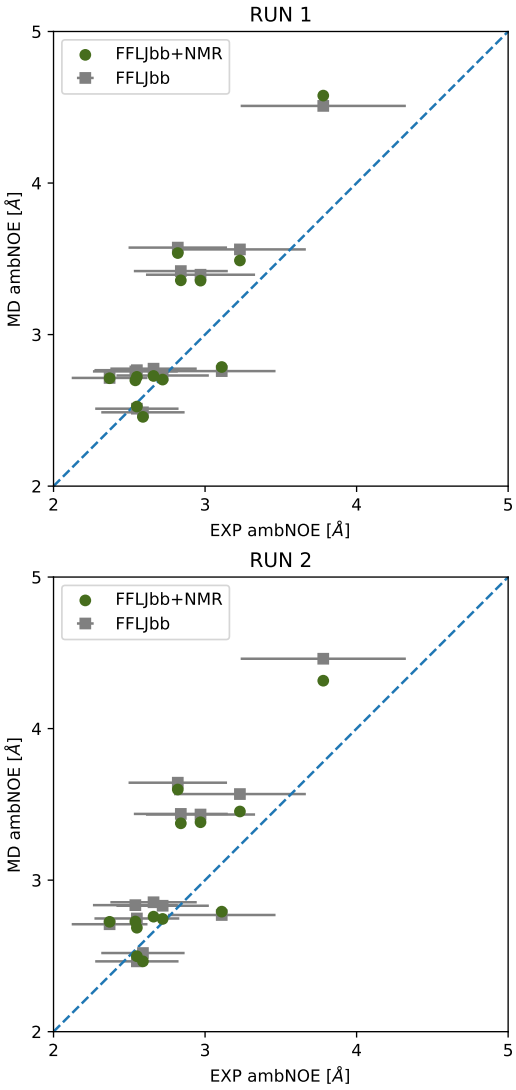
SI2: Cluster populations of two independent MD simulations using the FFLJbb force field.



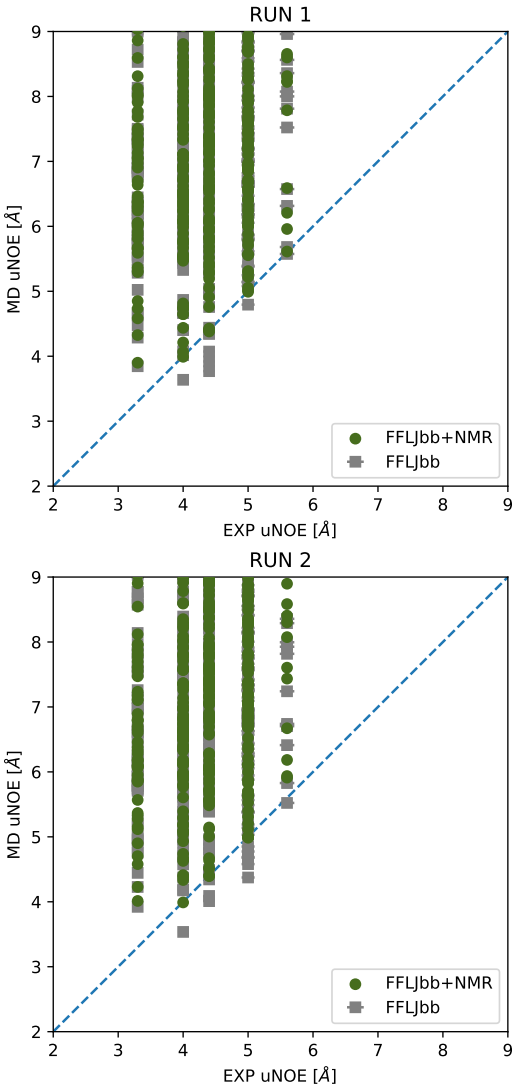
SI3: FARFAR2 cluster analysis. Clustering was performed as described in the Methods section, using kmeans clustering based on heavy atom RMSD to all residues. The top six out of ten clusters' representative structures are shown, representing 24.3 %, 21.5 %, 21.5 %, 14.7 %, 5.9 %, and 5.3 % of the ensemble. Residues are colored by rainbow from U1 in purple to C6 in red.



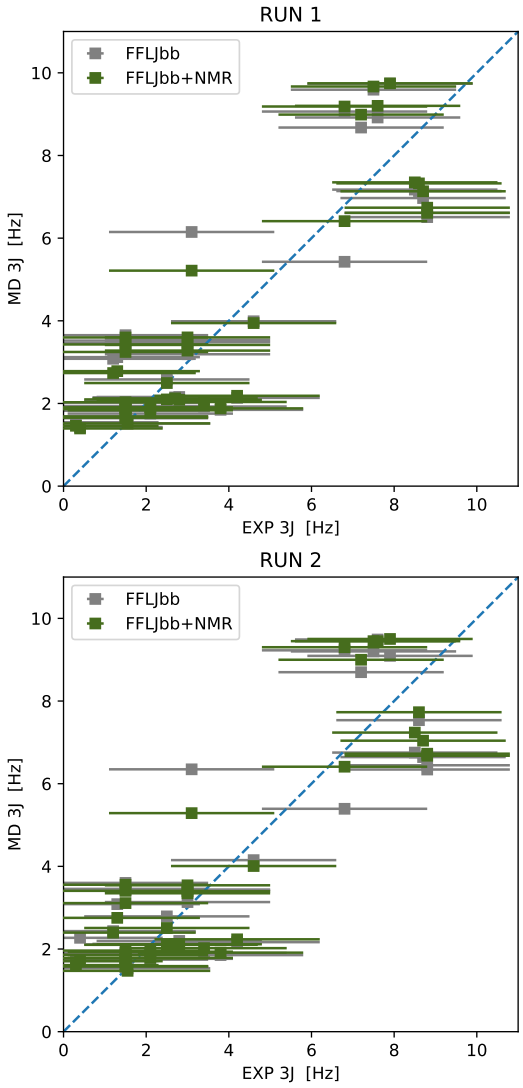
SI4: Experimental versus calculated NOE from FFLJbb ensemble. Values from run 1 and run 2 are reported. The dashed line indicates the diagonal.



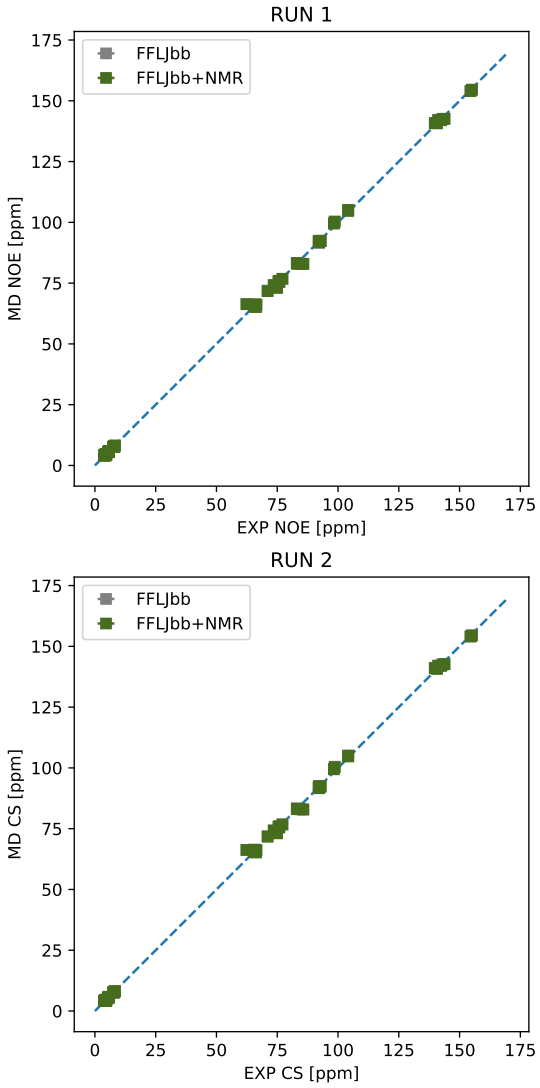
SI5 Experimental versus calculated ambiguous NOE from FFLJbb ensemble. Values from run 1 and run 2 are reported. The dashed line indicates the diagonal.



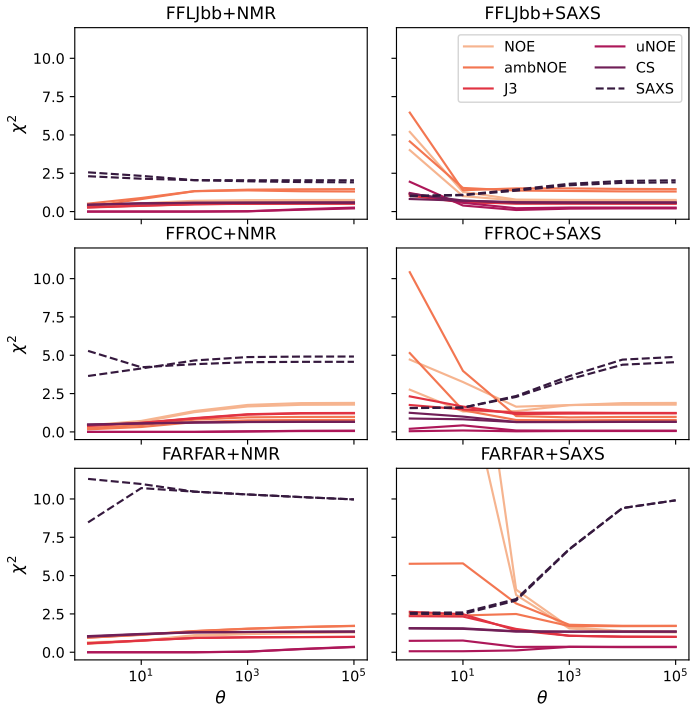
SI6 Experimental versus calculated unobserved NOE from FFLJbb ensemble. Values from run 1 and run 2 are reported. Points below the diagonal, shown as a dashed line, are uNOE violations.



SI7 Experimental versus calculated ^{3}J scalar couplings from FFLJbb ensemble. Values from run 1 and run 2 are reported. The dashed line indicates the diagonal.



SI8 Experimental versus calculated chemical shifts from FFLJbb ensemble. Values from run 1 and run 2 are reported. The dashed line indicates the diagonal.



SI9 χ^2 values as a function of the regularization parameter θ. In the left column, only NMR data are used for reweighting, but not SAXS. In the right column, SAXS data is used for reweighting, but not NMR data. The behavior for all three methods and for both replicates is reported.