(Please include how distance and torsion angle restraints were obtained at the beginning - these were provided by you. My guess is that distance - from your NOE spectra & torsion angle - I just used the same restraints in Sebastian's folder. I guess he generated them from chemical shift based TALOS prediction, but please make sure. He did not described in the JACS paper.)

Using distance and torsion angle restraints, a total of 100 structures for each sugar group (?) were refined by restrained molecular dynamics simulated annealing using the AMBER 11 software package (Case DA et al, 2010). These structures were subjected to 2,000 steps of energy minimization, followed by 20 ps of simulated annealing using a generalized Born solvent model (Tsui V & Case DA, 2000) and finally 2,000 steps of energy minimization. During the simulated annealing, the system was heated to 1,000 K for the first 2 ps, followed by 4 ps at constant temperature, and final cooling to 0 K for the remaining 14 ps. Force constants were 30 kcal mol−1 Å−2 for NOE restraints and 500 kcal mol−1 rad−2 for dihedral angle restraints. The 20 lowest energy structures were selected and analyzed using PROCHECK-NMR (Laskowski RA et al, 1996).

D.A. Case, T.A. Darden, T.E. Cheatham, III, C.L. Simmerling, J. Wang, R.E. Duke, R. Luo, R.C. Walker, W. Zhang, K.M. Merz, B. Roberts, B. Wang, S. Hayik, A. Roitberg, G. Seabra, I. Kolossváry, K.F. Wong, F. Paesani, J. Vanicek, J. Liu, X. Wu, S.R. Brozell, T. Steinbrecher, H. Gohlke, Q. Cai, X. Ye, J. Wang, M.-J. Hsieh, G. Cui, D.R. Roe, D.H. Mathews, M.G. Seetin, C. Sagui, V. Babin, T. Luchko, S. Gusarov, A. Kovalenko, and P.A. Kollman (2010), AMBER 11, University of California, San Francisco. (Sorry for the inconsistency of the format of names. I just copied it from somewhere. Please, let your citation software handle it.)

Tsui V, Case DA (2000) Theory and applications of the generalized Born solvation model in macromolecular simulations. Biopolymers 56: 275–291. doi: 10.1002/1097-0282(2000)56:4<275::aid-bip10024>3.0.co;2-e

Laskowski RA, Rullmannn JA, MacArthur MW, Kaptein R, Thornton JM (1996) AQUA and PROCHECK-NMR: programs for checking the quality of protein structures solved by NMR. J Biomol NMR 8: 477–486. doi: 10.1007/bf00228148