

Yet more about HBonding

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The current task is to decide whether or not it was likely that a water molecule was an H-bond bridge between the GalNAc N-H and the backbone O=C. If everything were lined up as indicated below, then the N — O distance should be, at max, 6 Å.

N-H ... O-H ... O=C

The minimum reasonable N — O distance should be 3 Å. If it is that distance, then it is likely that the N and O are directly H-bonded.

There are also many other things to gather from the data. cpptraj and/or ptraj can do some of it, but I have a library... it's just as easy to do it all myself.