

Shared H-bond

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I wrote the program required for the last post. It's attached here. I think the evidence is pretty good that there is a persistent shared H-bond in the GalNAc moieties. The hydrogen from the NAc is shared between the glycosidic O and the O in the peptide backbone. Here is a plot of the O — H — O angle versus the sum of the H — O distances. A typical H-bond distance is anything within about 3 Angstroms. So, if the sum of the distances stays under or near 6 A most of the time, with an angle less than 100 for O—H—O, that looks like a shared H to me. David says there aren't really any standards for it.

[do GalNAc analysis](#)

