I also found a couple of examples of macrocycles that are a hybrid between peptides and organic molecules. One such example is thiostreption (PDB **2L2Z** and **2L2X**, <https://onlinelibrary.wiley.com/doi/full/10.1002/anie.201003582>). I think this would be a good test case because of the complexity of the molecule. The NMR ensemble was calculated with CNS and according to the author it compares well with the Xray structure (PDB 1E9W).

These peptides sample a variety of lengths, linkages, methods used for the structures calculations and, to some extent, types of non-natural amino acids. I also included a stapled peptide.

-Paola