# ELECTRONIC SUPPLEMENTARY MATERIAL

## Structural Constraints for the Crh Protein from Solid-State NMR Experiments

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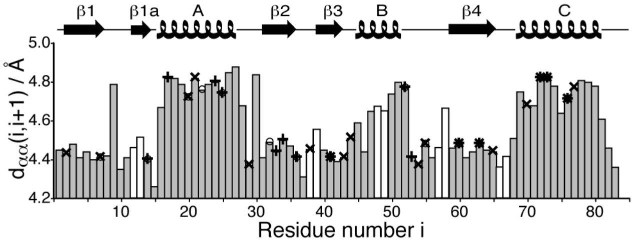

***Figure ESM 11.*** Sequential H$^{\alpha}$-H$^{\alpha}$ distances $d_{\alpha\alpha}(i,i+1)$ according to the crystal structure (bars) and sequential H$^{\alpha}$-H$^{\alpha}$ contacts identified in CHHC spectra recorded at 700 MHz with a ($^1$H,$^1$H) mixing time of 100 µs (×), 200 µs (○) and 300 µs (+). White bars represent the mean value of the two distances $d_{\alpha\alpha}(i,i+1)$ for contacts involving glycine residues.

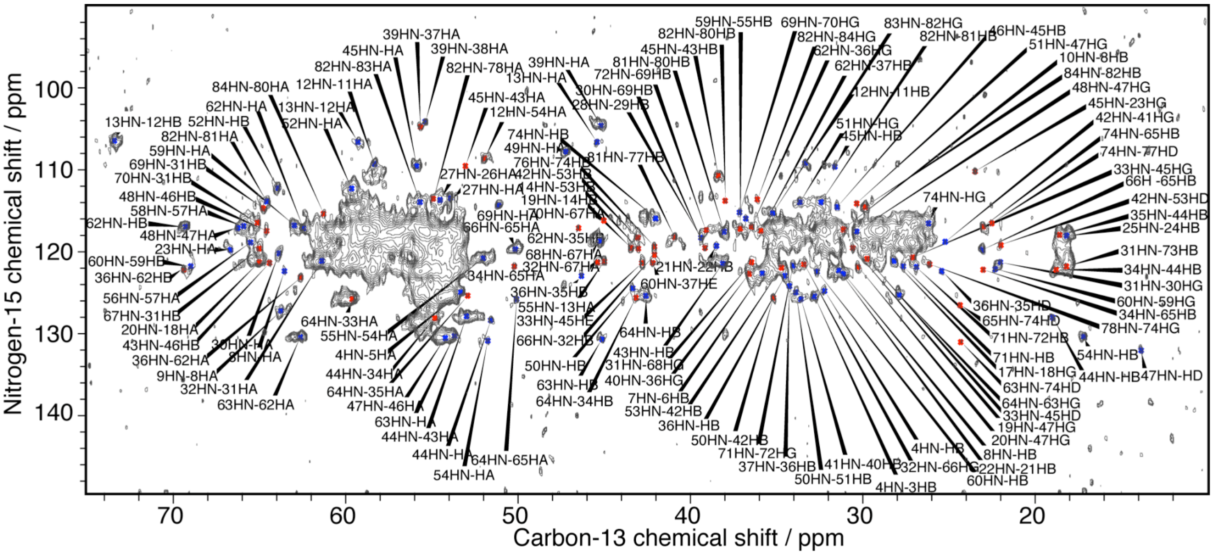

***Figure ESM 12.*** NHHC spectrum recorded with a mixing time of 100 µs. Intra-residue and sequential contacts are indicated in blue, medium- and long-range contacts in red.

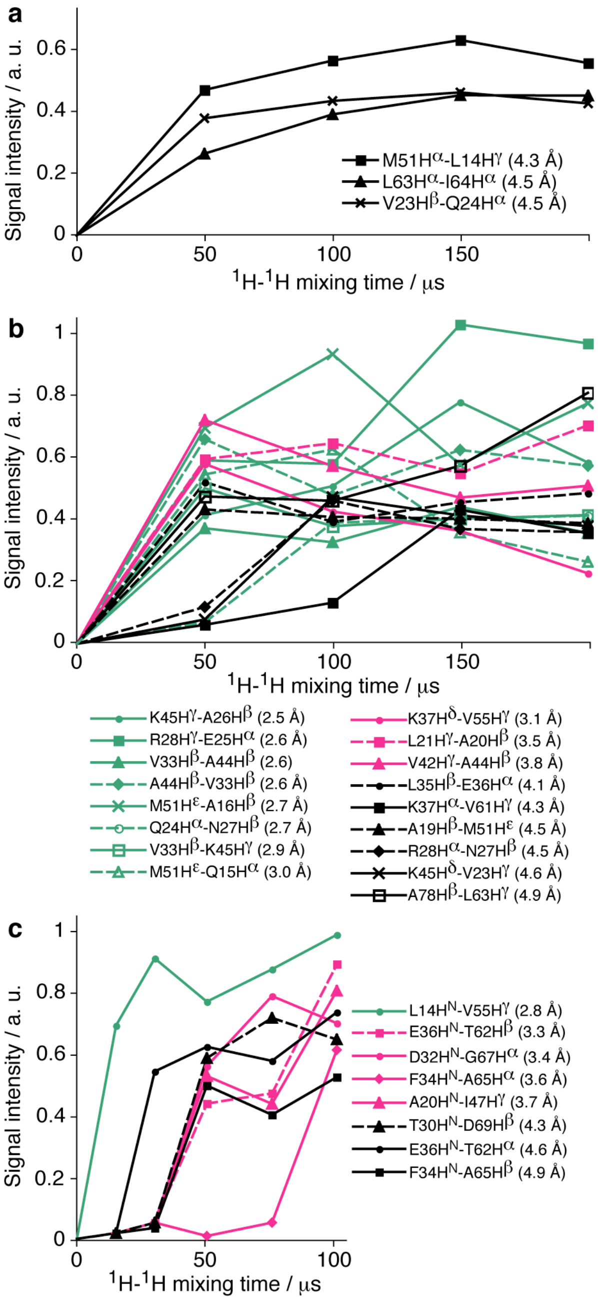

***Figure ESM 13.*** Magnetization build-up curves for inter-residue $^1$H-$^1$H contacts identified in spectra recorded at 500 MHz: CH···HC contacts involving carbon atoms with only one proton attached (a); other CH···HC contacts involving at least one carbon atom with more than one proton attached (b); NH···HC long-range contacts (c). Green curves correspond to $^1$H-$^1$H distances shorter than 3 Å, pink curves to distances between 3 and 4 Å, black curves to distances longer than 4 Å.

All the identified contacts involving carbon atoms with only one proton attached (Figure 13a) correspond to similar $^{1}$H-$^{1}$H distances and their build-up curves look very similar. Figure 13b exemplifies the case of multi-spin contacts in CHHC spectra: for the case of contacts involving carbon atoms with more than one proton attached, no clear correlation between the initial slope or the shape of the build-up curves and the $^{1}$H-$^{1}$H distance is observed any more. Figure 13c shows magnetization build-up curves for resolved long-range contacts in NHHC spectra. Even if for some contacts heteroatoms with only one attached proton are involved, no clear correlation to the inter-nuclear distance can be observed.

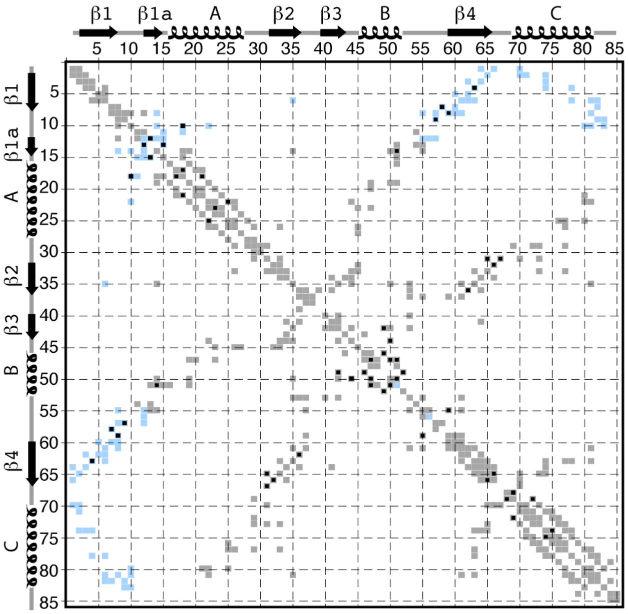

***Figure ESM 14.*** Predicted intra-monomer (grey) and inter-monomer (light blue) contacts, as well as missing signals (black, intra-monomer; blue, inter-monomer) in the spectrum recorded at 500 MHz with 150 μs mixing time, all corresponding to $^{1}$H-$^{1}$H distances smaller than 4 Å. Missing contacts involving methyl groups or arginine and lysine side chains were omitted. Indicated amino acids show at least one missing contact. Missing signals in the CHHC spectrum seem to concentrate around helix B and beta-strand 1a.