

# L-Isoleucyl-L-asparagine: a hybrid hydrogen bonding pattern

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## Supplementary material

Fig. 1S. Overlays between the two peptide molecules in the asymmetric unit. Molecule A is coloured in light blue, molecule B in black. (a) Overlay of all non-H atoms, RMS = 1.155 Å. (b) Overlay excluding the terminal amide group of the L-Asn side chain (shown in pale white for molecule A), RMS = 0.547 Å.

Fig. 2S. The two modes of water inclusion in the asymmetric unit. Neighbouring peptide molecules (in wireframe style) have been included to illustrate the hydrogen bonds formed by the water molecules.

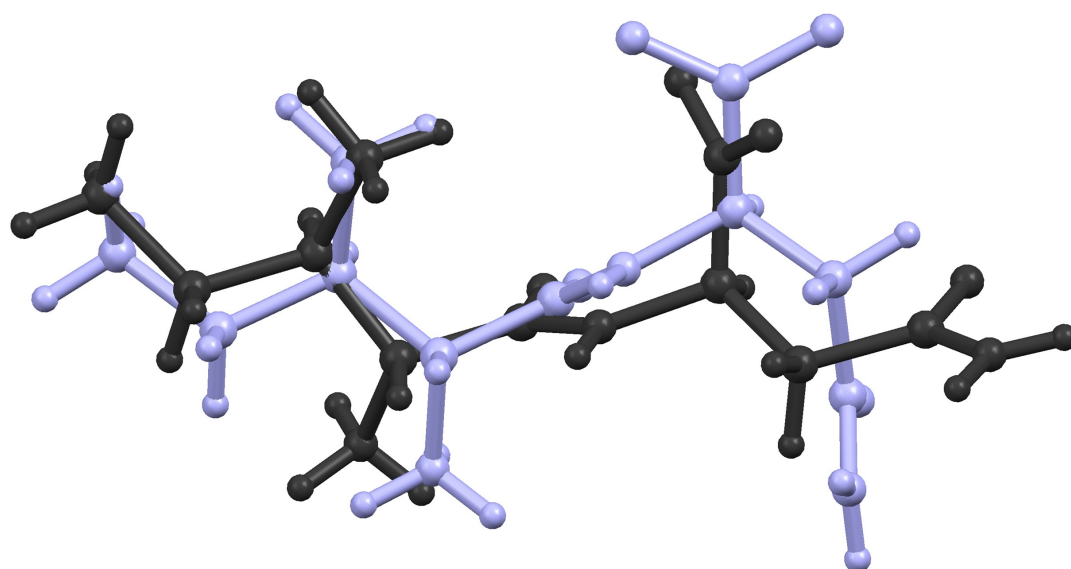
Fig. 3S. Location of water molecules in neighbouring unit cells along the 4.7855(4) Å *a*-axis. The major hydration pattern (white bars) can exist in two adjacent cells, and also a major and a minor pattern (grey bars), but not two minor patterns as this would give a too short 1.517 Å distance between O3W and O4W (arrow).

Fig. 4S. Detail of the hydrogen bonding between O2W and the carboxylate group of peptide molecule A. When this hydrogen bond is not present (minor hydration pattern, Fig. 2S), the carboxylate group rotates slightly to take a more coplanar conformation relative to N2A (O atoms in violet).

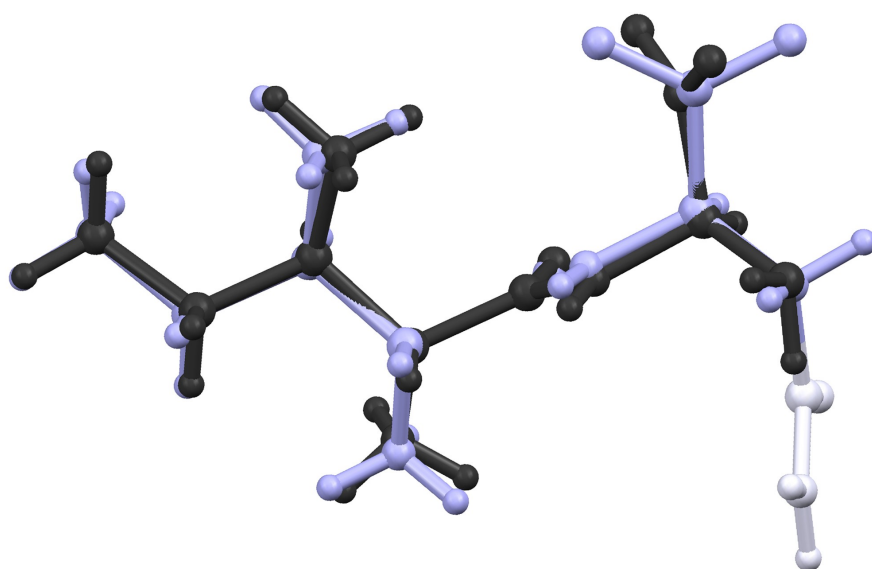
Fig. 5S. Hydrogen bonds in chains of (a) peptide A molecules and (b) peptide B molecules. H-atoms of the L-Leu side chains have been omitted. The grey ellipses emphasize side chain hydrogen bonds that add to the main chain hydrogen bonding shown in Fig. 3. (c) Chains of peptide molecules generated by main chain and side chain amide hydrogen bonds in the structures of L-Ser-L-Asn (Görbitz & Hartviksen, 2008) and (d) L-Met-L-Asn (Stievater & Srikrishnan, 2005).

## References

- Görbitz, C. H. & Hartviksen, L. M. (2008). *Acta Cryst.* **C64**, o171-o176.  
Stievater, T. & Srikrishnan, T. (2005). *J. Chem. Cryst.* **35**, 529-533.



a)



b)

Fig. 1S

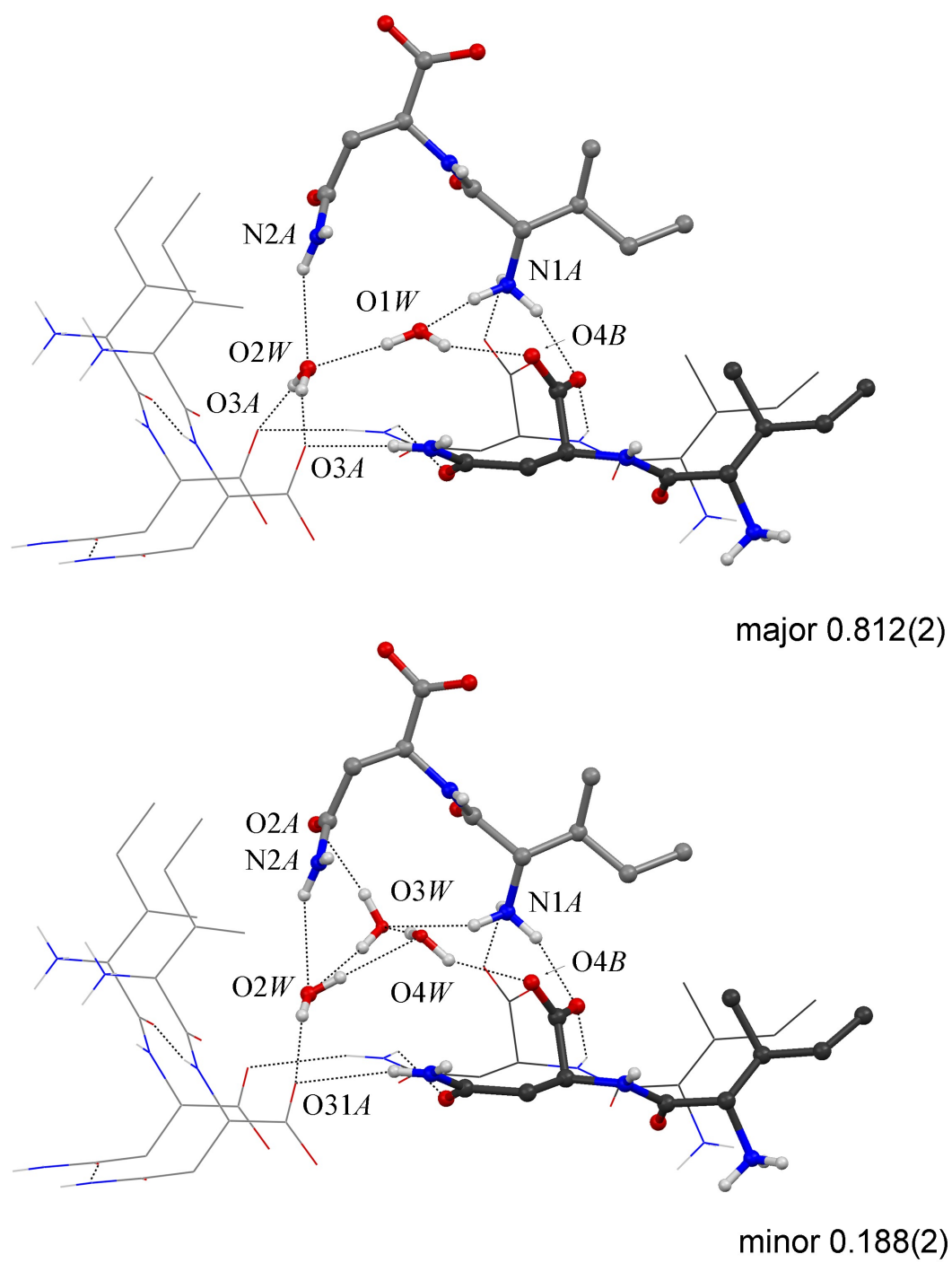


Fig. 2S

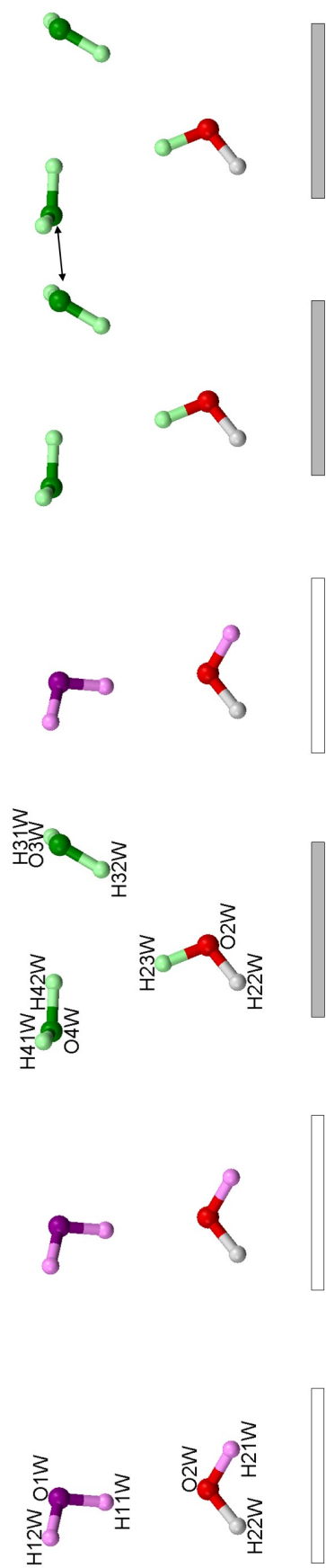


Fig. 3S

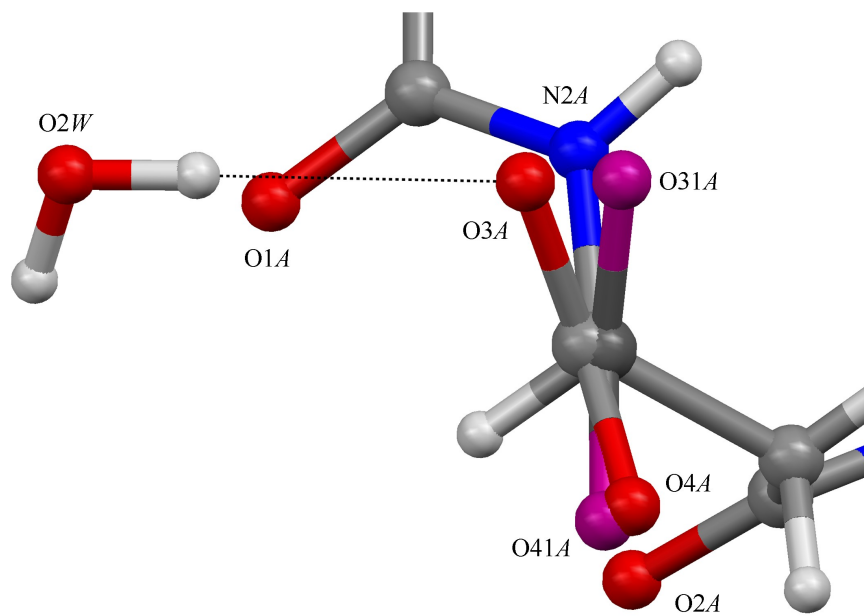


Fig. 4S

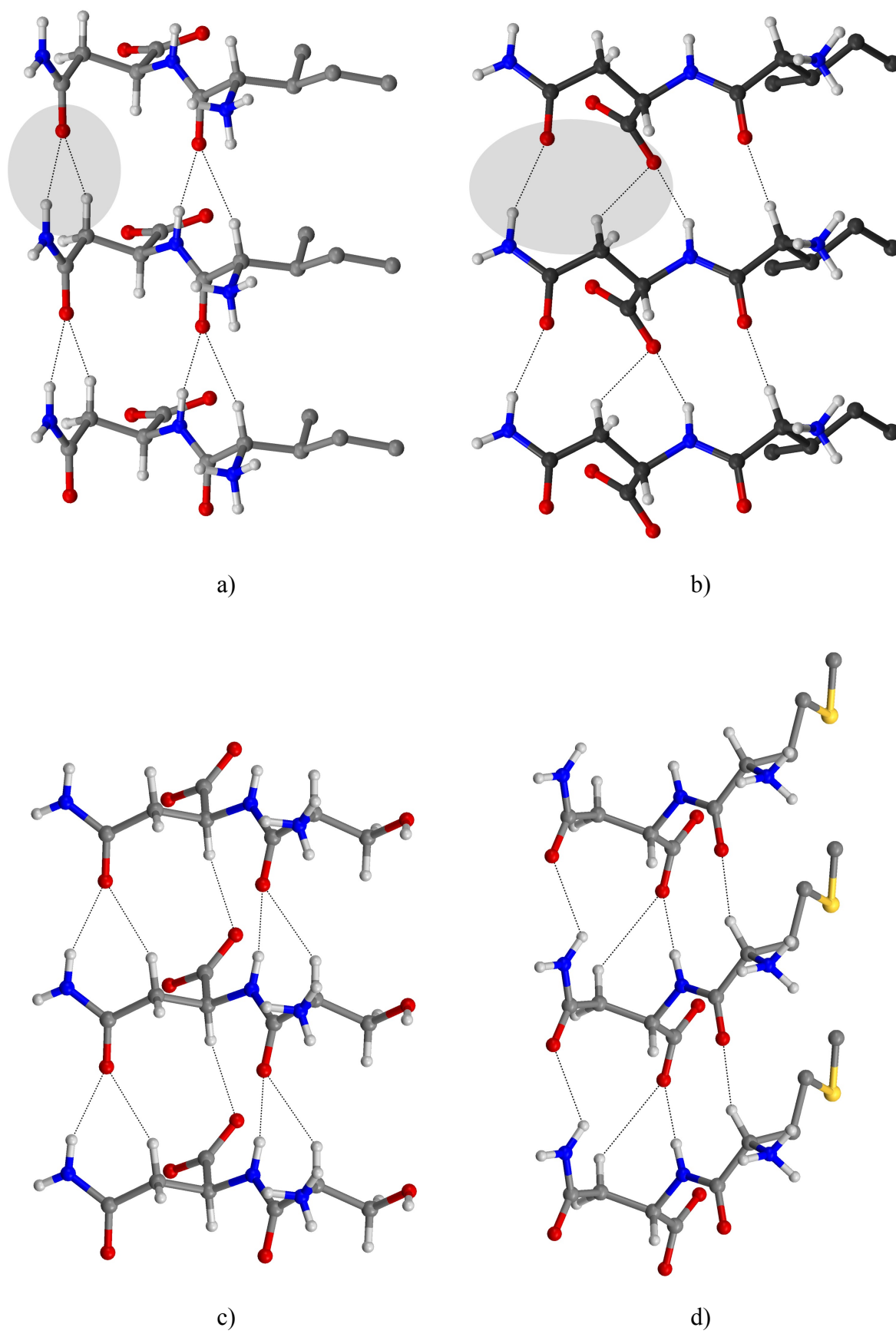


Fig. 5S