Supporting Information for

" Pseudoracemic amino acid complexes: blind predictions for flexible two-component crystals "

Supporting Information contains:

1) CIFs of the three experimentally determined crystal structures.
2) Additional packing diagrams of predicted and observed packing patterns of amino acid complexes.
3) A CIF structure file of the 20 lowest energy predicted structures is provided for each complex, with structures given in order of increasing energy.

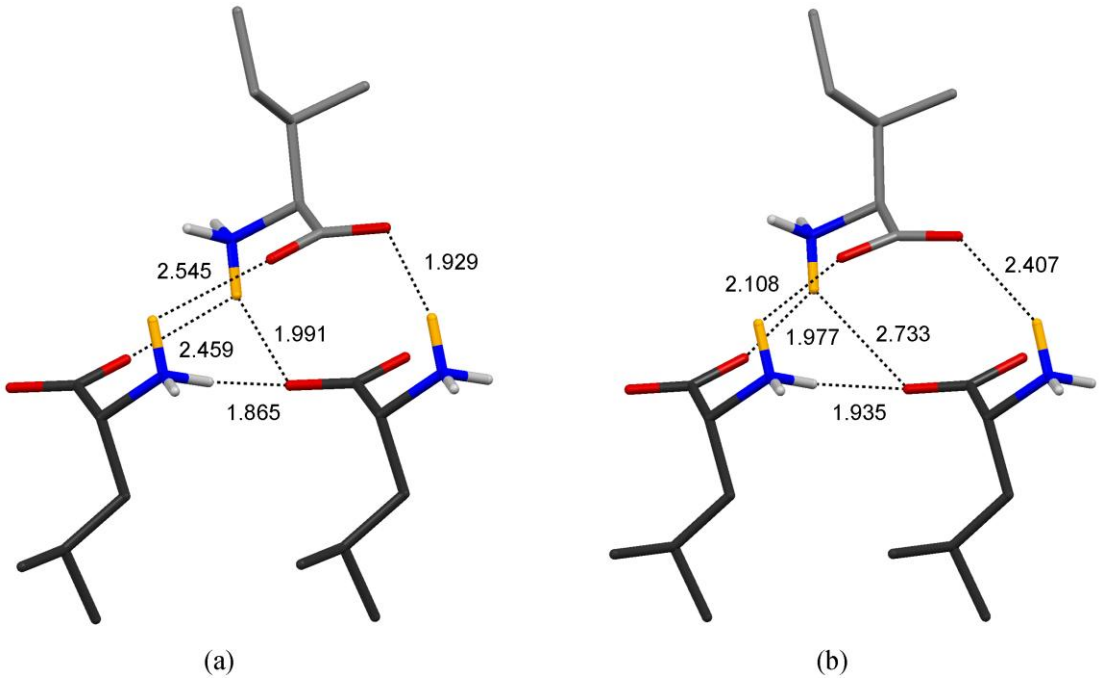

Fig. S1. Hydrogen bonding detail in the L-*a*Ile:D-Leu complex (I) (a) in the crystal and (b) in the #1 predicted model. A minor shift in the relative positions of the two sheets constituting a layer act to switch the minor components of three-centre interactions (H atoms coloured in yellow) in the experimental structure into the major component in the theoretical structure. N-H distances for the X-ray structure have been normalized to 1.035 Å, the length used for these bonds in calculations.

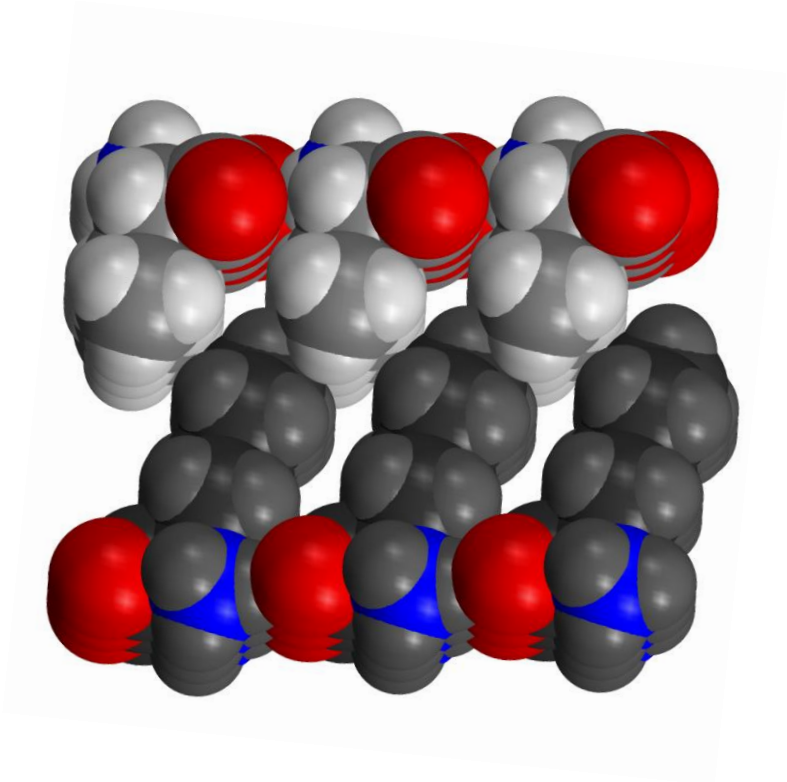

Fig S2. “Knobs-in-holes” fit between side chains in the crystal structure of L-Abu:D-Nle complex (III). C and H atoms of D-Nle are shown in dark grey colour.

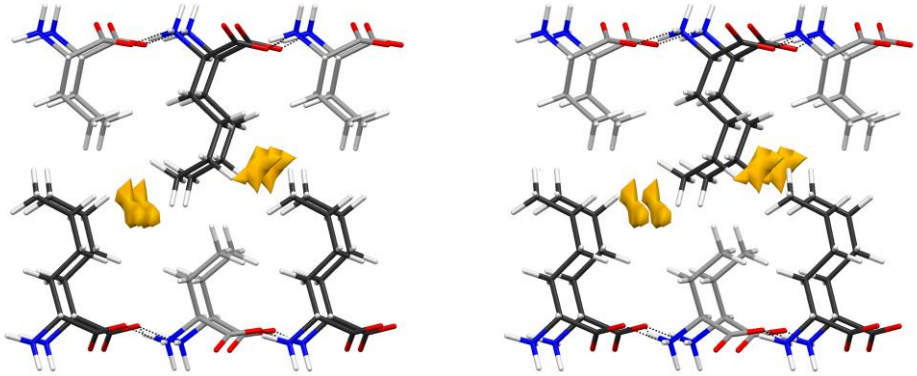

Fig. S3. Stereo drawings of (a) the #36 LD-LD structure of complex III. Voids coloured in orange (calculated using a 0.8 Å probe radius with 0.4 Å grid spacing) are smaller than for the #29 structure due to a folded rather than straight D-Nle side chain.

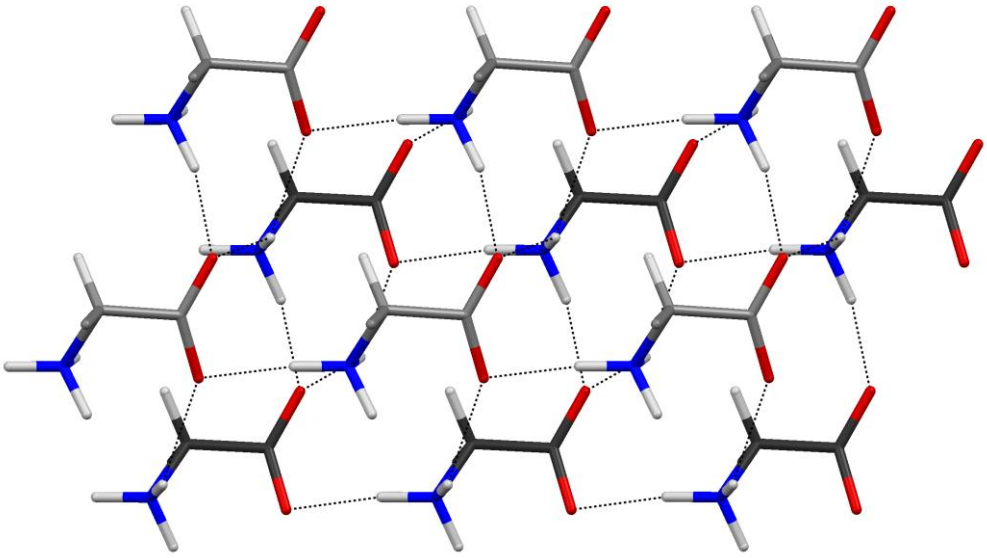

Fig. S4. Construction of a pL1-D1 layer predicted for all three complexes, but never found experimentally. The upper layer (C-atoms in light grey) is the same as in Fig. 1, but the bottom layer (D-amino acid, C-atoms in dark grey) is parallel to the first one rather than antiparallel as in observed L1-D1 structures.

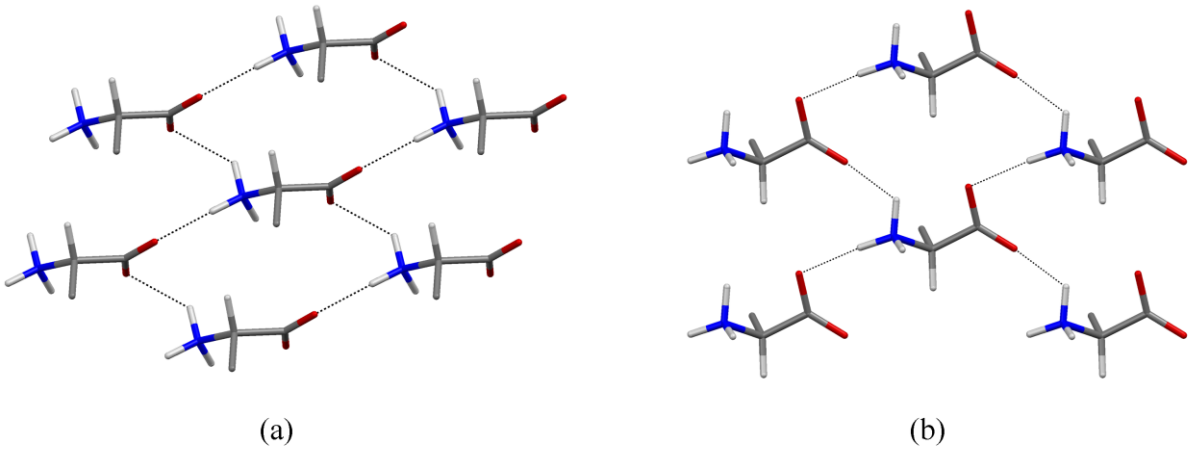

Fig S5. (a) Individual L4 sheet from the #2 predicted model of complex (III). (b) Individual L5 sheet of the #12 predicted model of complex (II). The sixteen-membered hydrogen-bonded ring system of the L1 sheet (Fig 1) is retained in both the L4 and the L5 sheet, but the rings are perturbed in order to fit either a L4 sheet to a D4 sheet, or a L5 sheet to a second L5 sheet.

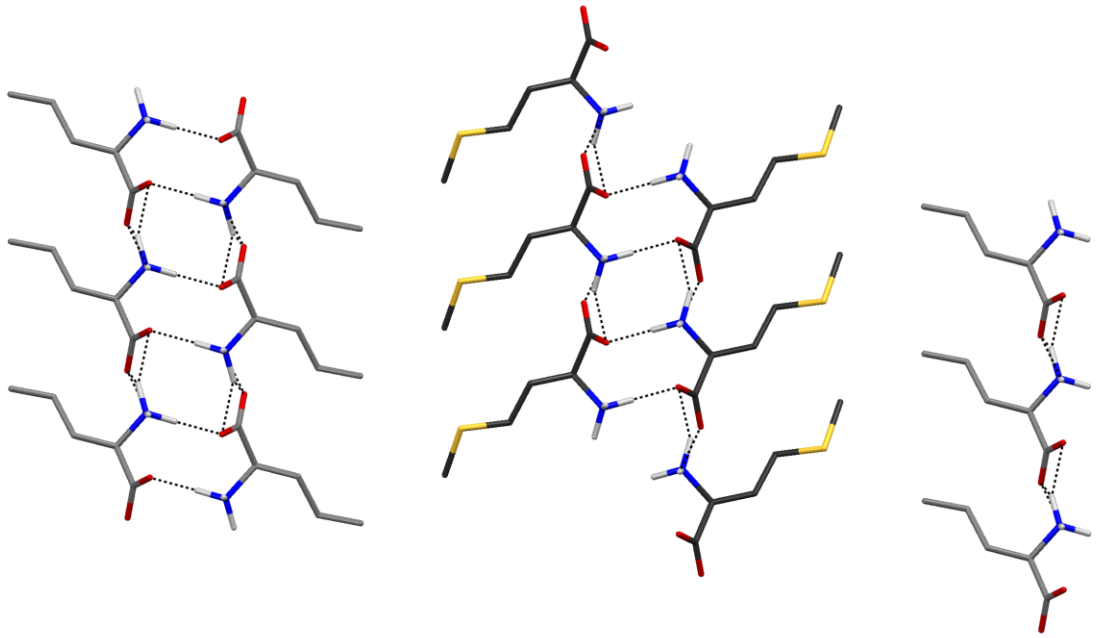

Fig. S6. The #12 structure of complex (II) where amino acids are separated into two independent hydrogen-bonding regions with a L5-L5 layer for L-Nva and a D5-D5 layer for D-Met.

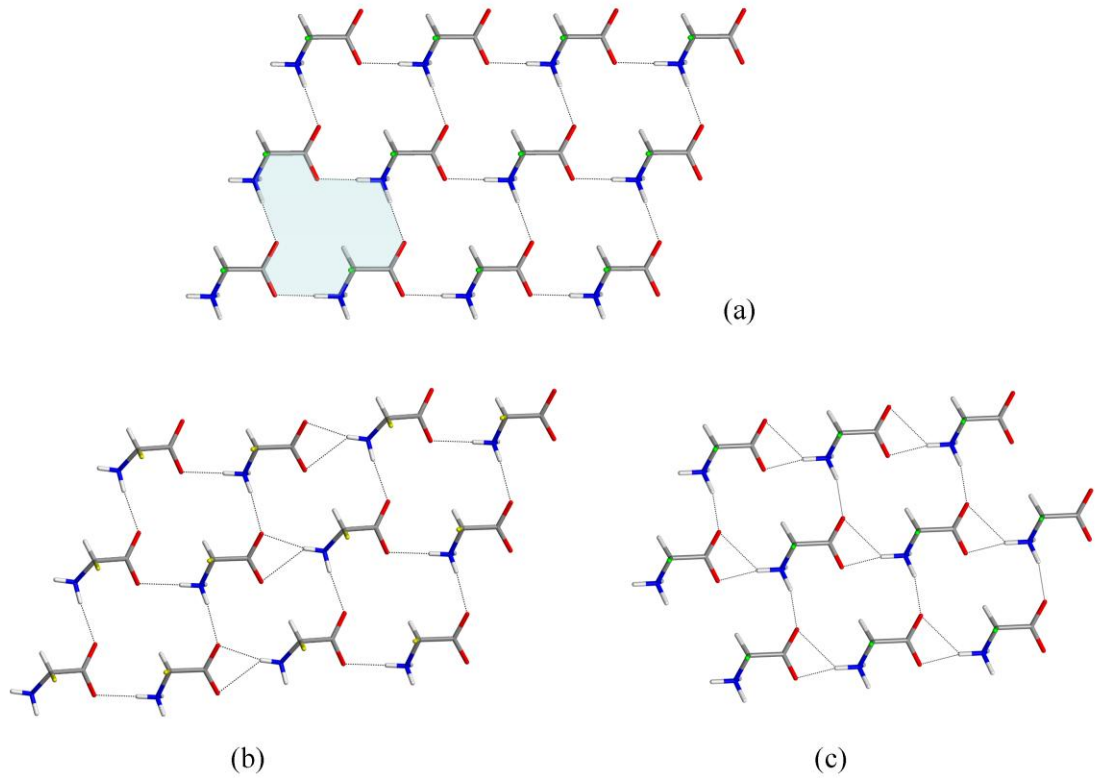

Fig. S7. The (a) L1 sheet observed for both (pseudo)racemic and enantiopure amino acid structures together with the (b) L2 and (c) Lx sheets found exclusively in homochiral structures. The typical sixteen membered ring system highlighted in (a) is also found in (b), but the second hydrogen-bonded ring systems (these structures have $Z` = 2$) is modified through a shift of carboxylate acceptor atom for the N-H…O (syn) interaction. The ring in the Lx sheets can be seen as an average between the two rings of the L2 sheet.