SOLVING THE STRUCTURES OF LIGHT-ATOM COMPOUNDS WITH POWDER CHARGE FLIPPING

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Supplementary Information

β-peptide TY-174

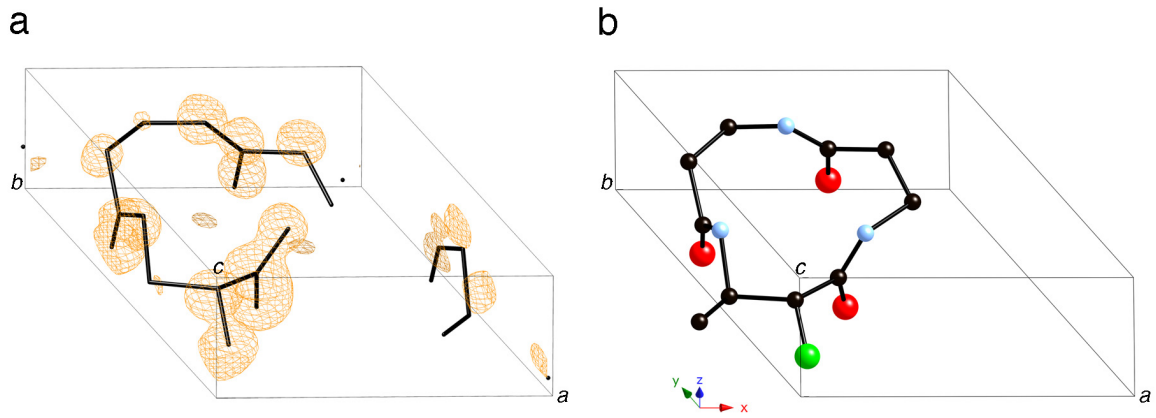

Figure S1 (a) Electron density map from *Superflip* for TY-174 with the all-carbon model obtained from the automatic interpretation by EDMA superimposed (b) The trial molecular structure derived from (a) used to start the Rietveld refinement. Carbon – grey, nitrogen – blue, oxygen – red, fluorine – green

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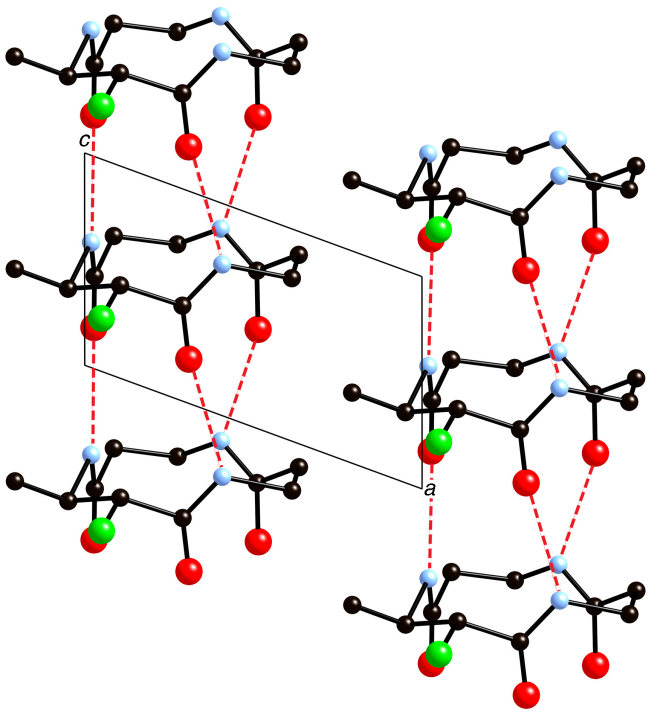

Figure S2. Refined crystal structure of TY-174 showing the stacking of the molecules along the *c* axis. Hydrogen atoms have been omitted for clarity.

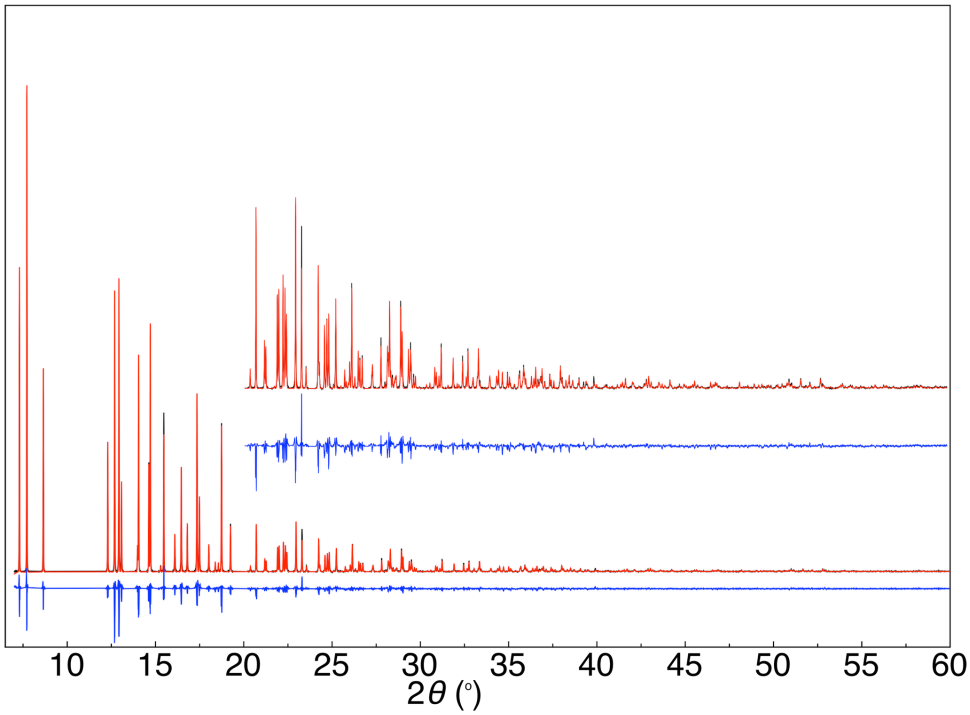

Figure S3. Results of the Rietveld refinement for TY-174. Black, red and blue correspond to observed, calculated and difference profiles, respectively. The pattern in the inset has been scaled up by a factor of 6 to show more detail.

β-peptide TY-120

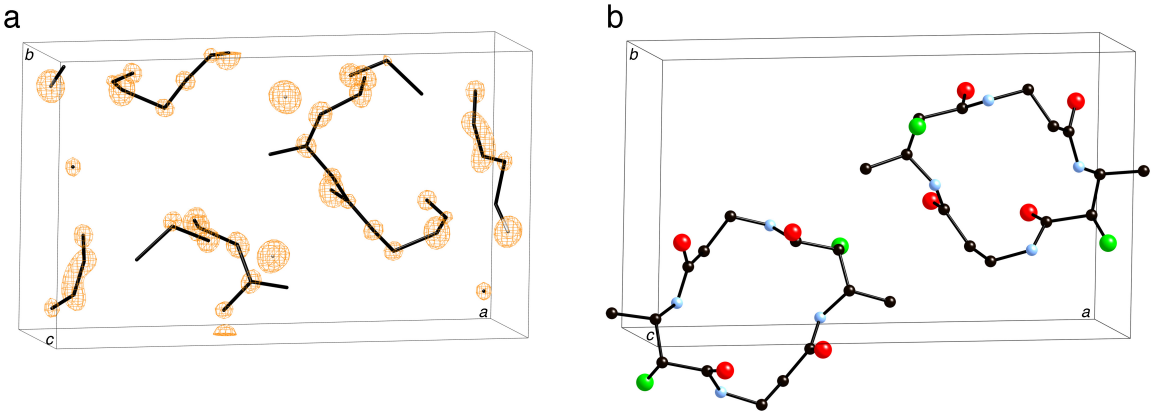

Figure S4. (a) Electron density map from *Superflip* for TY-120 with the all-carbon model obtained from the automatic interpretation by EDMA superimposed (b) The trial molecular structure derived from (a) used to start the Rietveld refinement. Carbon – grey, nitrogen – blue, oxygen – red, fluorine – green

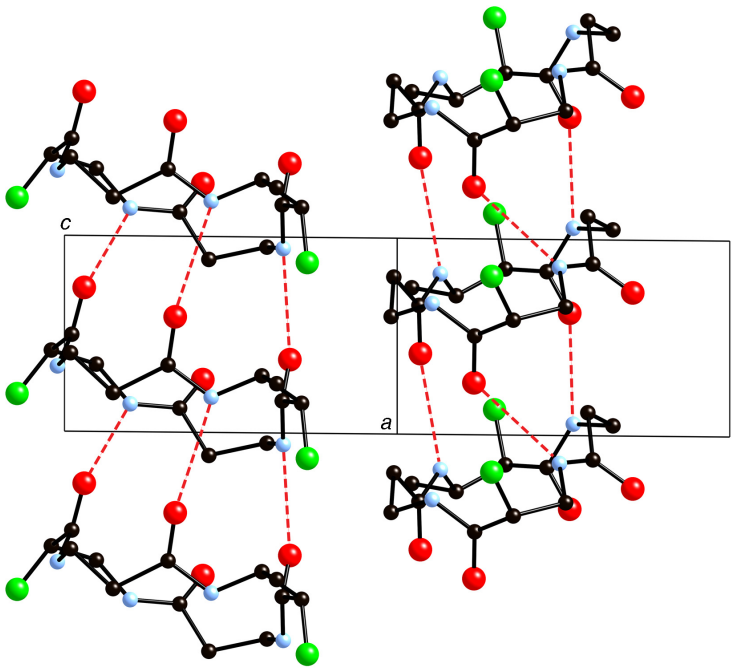

Figure S5. Projection of the refined crystal structure of TY-120 along the [-110] direction showing the stacking of the molecules along the *c* axis. Hydrogen atoms have been omitted for clarity

β-peptide TY-207

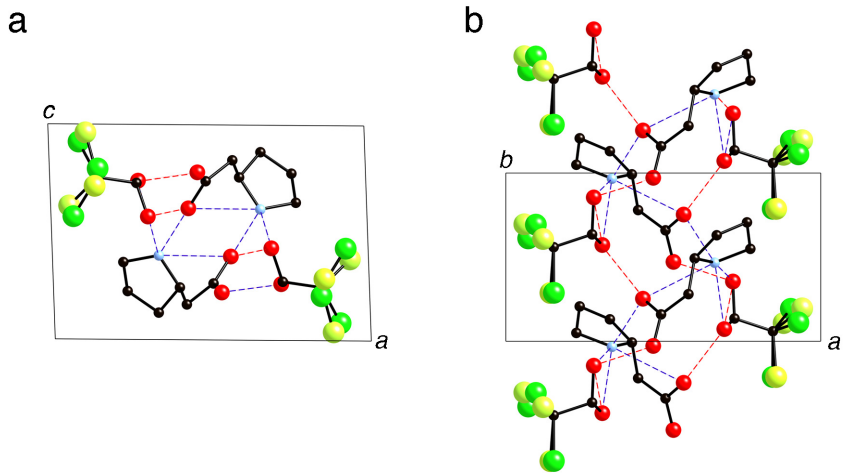

Figure S6. Projections of the refined crystal structure of TY-207 showing the hydrogen bonding scheme (a) along the [010] direction, and (b) along the [001] direction. All chlorine atoms are disordered with relative occupancies 0.5. The two disordered sets are shown in green and light green. Hydrogen atoms have been omitted for clarity.

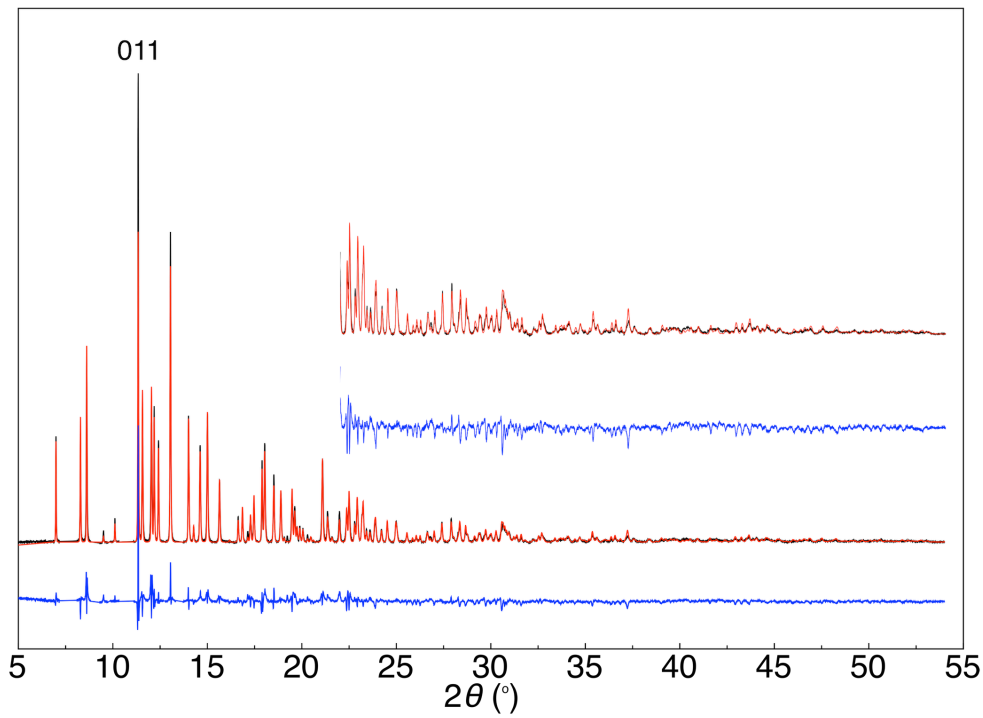

Figure S7. Results of Rietveld refinement for TY-207. Black, red and blue correspond to observed, calculated and difference profiles, respectively. The pattern in the inset has been scaled up by a factor of 6 to show more detail. The peak showing the highest discrepancy between the calculated and observed intensity corresponds to reflection 011