Experimental section

Materials

All chemicals and model compounds and solvents were purchased from HEOWNS biochemical technology co., LTD, China. In this work all reagents were used without further purification. Single crystal structures are obtained from Cambridge Structural Database (CSD).

Characterization

CD spectra were collected with an Applied Photophysics ChirascanV100. About 5 mg the above crystals were weighed, which was mixed with 500 mg KBr, followed by grinding into powders. 50 mg powders were weighed, followed by tableting into thin, transparent tablets, which were deposited to CD spectroscopy tests. Scanning electron microscope (SEM) images were attained by a Zeiss scanning electron microscope. The samples for SEM detection were dropped in the silicon pellet, dried and then sprayed by the gold. Powder X-ray diffraction (XRD) patterns were collected on a German Bruker/D8 Advanced diffractometer with Cu Kα radiation (λ = 0.15406 nm, voltage 40 KV, current 40 mA). The samples were casted onto cover glasses (18 mm × 18 mm) and dried to form thin films. Fourier transform infrared (FT-IR) measurements were performed on an Avatar 370 FT-IR spectrometer. Young's moduli were measured with a Bioscope Resolve atomic force microscopy (AFM).

Quantum mechanical calculation of ECD spectrum

Based on the time-dependent density functional theory (TDDFT) via the Gaussian 16 program. Calculation details could be found in the main text.

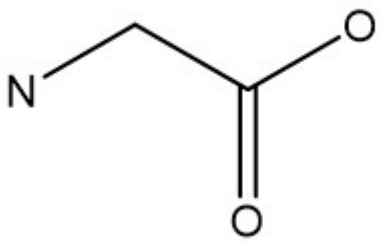

Figure S1. α-Amino acid backbone used for CCDC searching

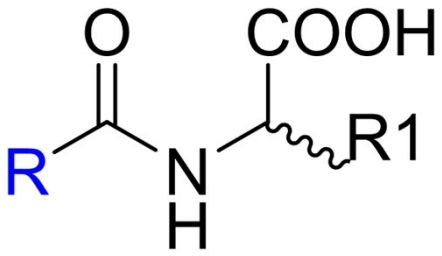

Figure S2. A generic chemical structure of N-protected amino acids

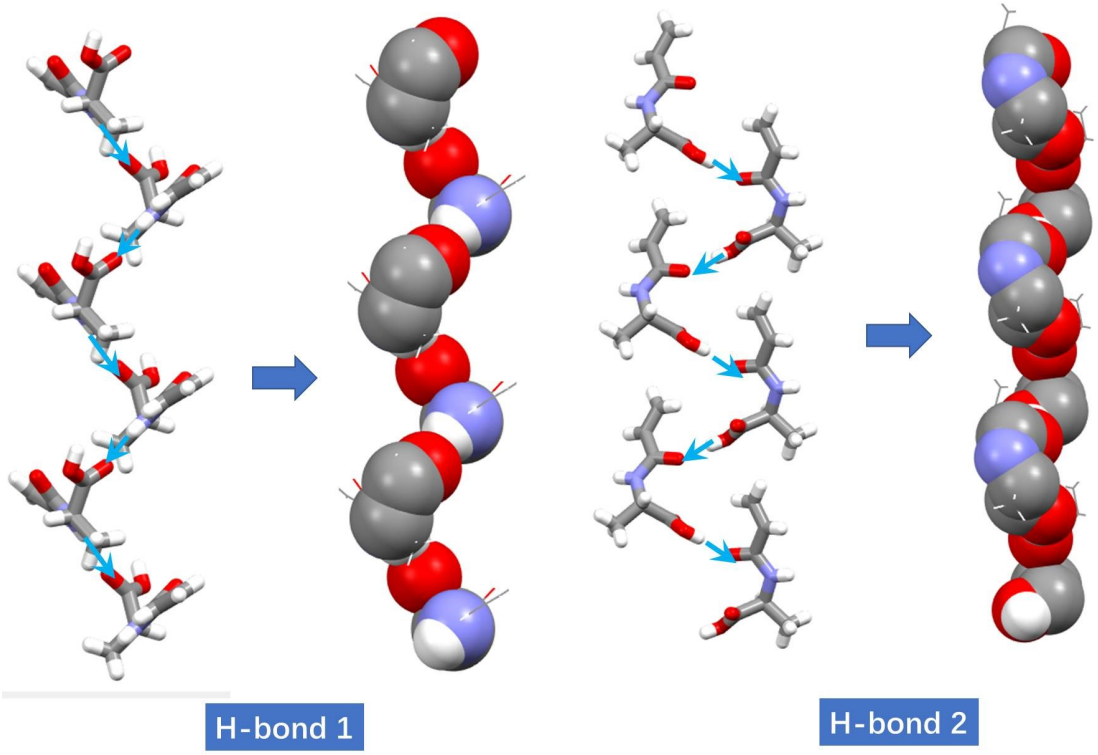

Figure S3. Two H-bond arrays induce the different chiral packing.