Supporting Information for

Microtubes with Rectangular Cross-Section by the Self-Assembly of a Short Helical β-Peptide Foldamer

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Materials

The synthesis of the $ACPC_4$ was performed by following the literature protocol.[1,2] All chemicals for the preparation of the $ACPC_4$ were purchased from Sigma Aldrich, Acros, Junsei, and TCI, and were used without further purification. High purity water was generated by Milli-Q apparatus (Millipore).

Self-Assembly Procedure

$ACPC_4$ was dissolved in a mixed solvent (1 mg mL^{-1}) of methanol (90%) and distilled water (10%) with slight sonication at room temperature, which yielded a transparent solution. 3 μL of $ACPC_4$ solution was dropcasted on Si (100) wafer, and dried under ambient condition till complete solvent evaporation. After about 5 min, white precipitation corresponding to microtubes with rectangular cross-section remained on surface.

Experimental Section

***Preparation of single crystal of $ACPC_4$*:** $ACPC_4$ was dissolved in a mixed solvent (3 mg mL^{-1}) of methanol (90%) and distilled water (10%) by applying vortexing at ambient temperature. The crystal solution was incubated at ambient temperature to induce slow evaporation. After 10 days, about 70% of the solvent remained and a few crystals were found at the bottom of the vial.

***Single crystal X-ray diffraction*:** Single crystal X-ray data for the $ACPC_4$ was collected on a Bruker SMART APEXII diffractometer equipped with graphite monochromatized MoKα radiation (λ = 0.71073 Å). The preliminary orientation matrix and cell parameters were determined from six sets of ω scans at different starting angles. Data frames were obtained at scan intervals of 0.5° with an exposure time of 10s per frame. The reflection data were corrected for Lorentz and polarization factors. Absorption corrections were carried out using SADABS. The structure was solved by a direct method and refined by full-matrix least-squares analysis using anisotropic thermal parameters for non-hydrogen atoms with the SHELXTL program. The following parameters were obtained for

$C_{36}H_{52}N_4O_7$: Mr = 652.82, triclinic, $P1$, a = 9.3019(7), b = 9.6426(7), c = 11.6855(7), α = 87.354(2), β = 89.943(2), γ = 61.196(2), V = 917.19(11) Å^3, Z = 1, ρ_{calc} = 1.182 g cm^{-3}, ρ_{exp} = 1.182 g cm^{-3}, μ =

0.082 mm^{-1} (corrected, Multi-Scan), F(000) = 352, θ_{max} = 28.23°, 14868 data collected, 7499 unique (R_{int} = 0.0463), 419 parameters, R_1 = 0.0716 (I> 2σ (I)), wR_2 = 0.2092 (all data), GOF = 1.033, Flack parameter = -0.7(17). CCDC 783791 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

NMR Spectroscopy**:** ^{1}H NMR spectra were recorded on a Bruker AVANCE II 900 spectrometer equipped with a cryogenic probe. $ACPC_4$ was dissolved in pyridine-d_5, and spectra were collected at 298K. Two-dimensional spectra (COSY, TOCSY and ROESY) were recorded employing standard pulse sequences with the number of acquisitions set to 2 for COSY, 8 for TOCSY, and 16 for ROESY, respectively. TOCSY spectra were recorded with mixing time of 60 ms. ROESY spectra were acquired with spin lock time of 300 ms. Proton assignments were made based on a combination of COSY, TOCSY and ROESY spectra.

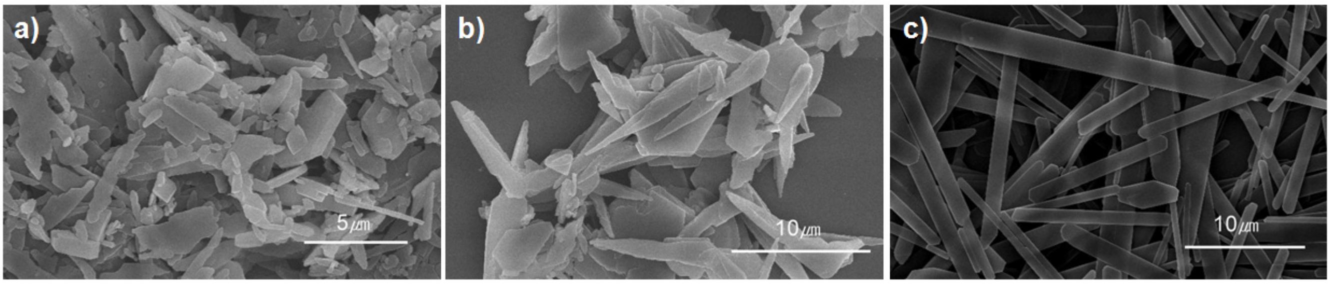
Characterization**:** SEM images were obtained by using a field-emission scanning electron microscope (FE-SEM, Hitachi S-4800, Japan) at an acceleration voltage of 10 kV after Pt coating (SCD 050 platinum evaporator, Bal-tec, Germany). TEM images were obtained by using a Tecnai F20 (Philips), field-emission transmission electron microscope (FE-TEM), at an acceleration voltage of 200 kV. The circular dichroism signal was measured with a Jasco-815 spectrometer (Jasco. Inc., Japan) by using methanolic solutions of $ACPC_4$. Sample cells with a path length of 1 mm were used. PXRD patterns were obtained from a multi-purpose attachment X-ray diffractometer (Rigaku, D / Max-2500) equipped with a pyrolytic graphite (002) monochromator. Characteristic Cu Kα radiation was used as an incident beam (λ=1.54178Å) and the diffraction patterns were scanned over 2θ values ranging from 3º up to 70º in increments of 0.02º at room temperature. Profile refinement of the structure model was performed via the Le Bail method with the GSAS package. The profile was matched in the 2θ range of 4– 70º because of the severe overlap of the peak at d < 1.4Å, and the poor signal to noise ratio of the data at very high angles. During the Rietveld refinement, a pseudo-Voigt/FCJ function, together with a manually interpolated background, was used to describe the peak shape.

***Ab initio* indexing and Rietveld refinement of PXRD pattern:** The X-ray diffraction pattern was indexed using the DICVOL04 program[3] implemented in the *Fullprof* program suite.[4] The obtained lattice parameters for the unit cell are a = 16.913 Å, b = 9.307 Å, c = 11.691 Å, α = 90.0°, β = 93.011° and γ = 90.0° in monoclinic symmetry with high FOM (20) = 59.2. These lattice parameters are different from those of the single crystal and show that the unit cell volume is doubled.

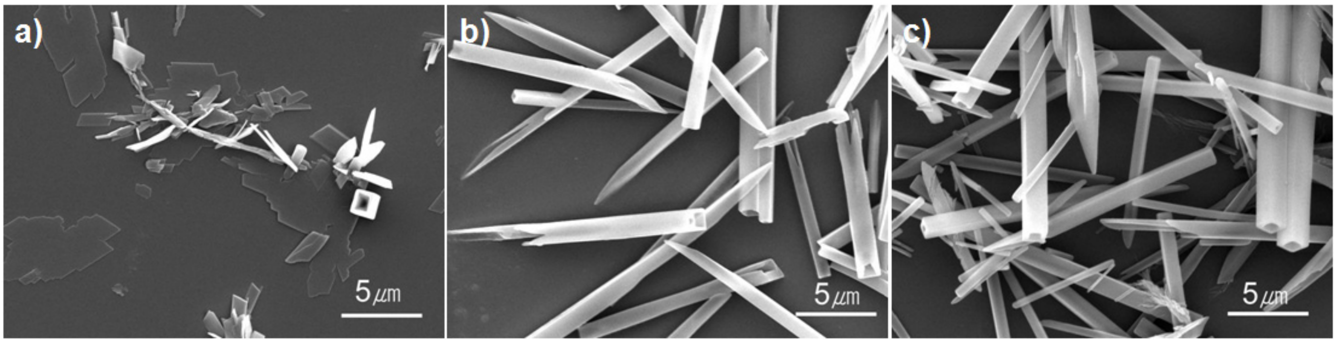
The Le Page analysis for the obtained cell parameters was performed to look for a better cell parameters.[4] The result suggested the presence of a triclinic conventional cell, a= 35.083 Å, b = 16.913 Å, c = 11.691 Å, α = 86.99°, β = 92.90° and γ = 164.62°. The corresponding triclinic cell parameters can be transformed to the standard form further, a = 9.3048 Å, b = 11.690 Å, c = 16.913 Å, α = 92.972°, β = 90.009° and γ = 90.043°. The final cell parameters were similar to those obtained from the peak indexing, while the crystal system was triclinic symmetry rather than monoclinic symmetry.

In order to get the initial structure, the global optimization was performed up to the resolution of d = 2.0 Å using the parallel tempering implemented in the *free object of X-ray crystallography*.[5] Prior to the optimization, the Le Bail fitting,[6] which is structureless parameter fitting, was performed to find the optimized profile parameters. At this stage, the result of the Le Bail fitting showed that the lowest R_{wp}, 4.78 % can be obtained using the $P1$ space group. At first, the structure taken from single crystal tetrapeptide as a rigid body was optimized without sacrificing the detail structure using parallel tempering where the number of trial runs was more than 2,000,000. Then, the obtained structure was considered as a flexible model with automatic constraints and optimized to achieve stable structure. The obtained structure was examined visually to check the overlap of chains or atoms. Through such procedure, the final obtained $P1$ space group gave non-overlapping stable optimized structure with the lowest R_{wp} and R_p values of 16.8 % and 12.5 %, respectively. The final obtained structure was used as the initial structure for the subsequent Rietveld refinement.

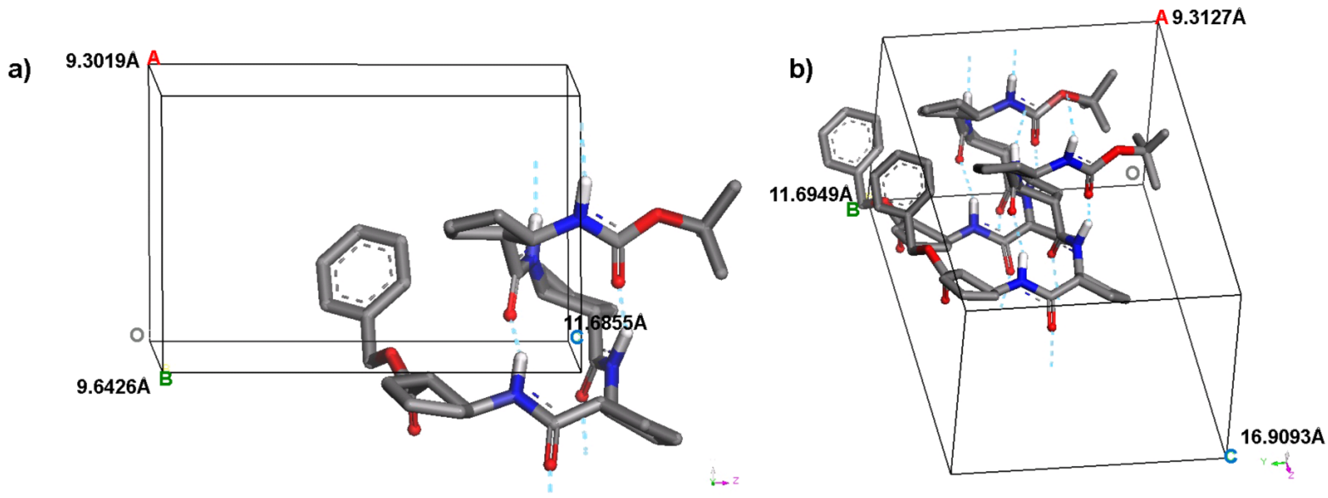
For the Rietveld refinement, the soft constraints were set for the $ACPC_4$ unit. The thermal displacement factor was set the same for all atoms. The C-C, C-N, C-O distances and all angles were restrained with a weighting factor of 50, initially.[7] The weighting factor was decreased progressively to 2.60 with the progress of the refinement.[8] Figure 3d shows the result of the final Rietveld refinement using the *GSAS* program suite.[8,9] Up to d = 1.4 Å, the final refinement had a reasonable fitting quality, R_{wp} = 6.57 %, R_p = 4.85 %, and R_F = 2.98 % (See Supporting Table S2). The detailed structural parameters are listed in Table S3 (Supporting Information). Most of the molecular modeling was carried out using MS modeling software package v 4.2 (Accelrys Inc.).[10]



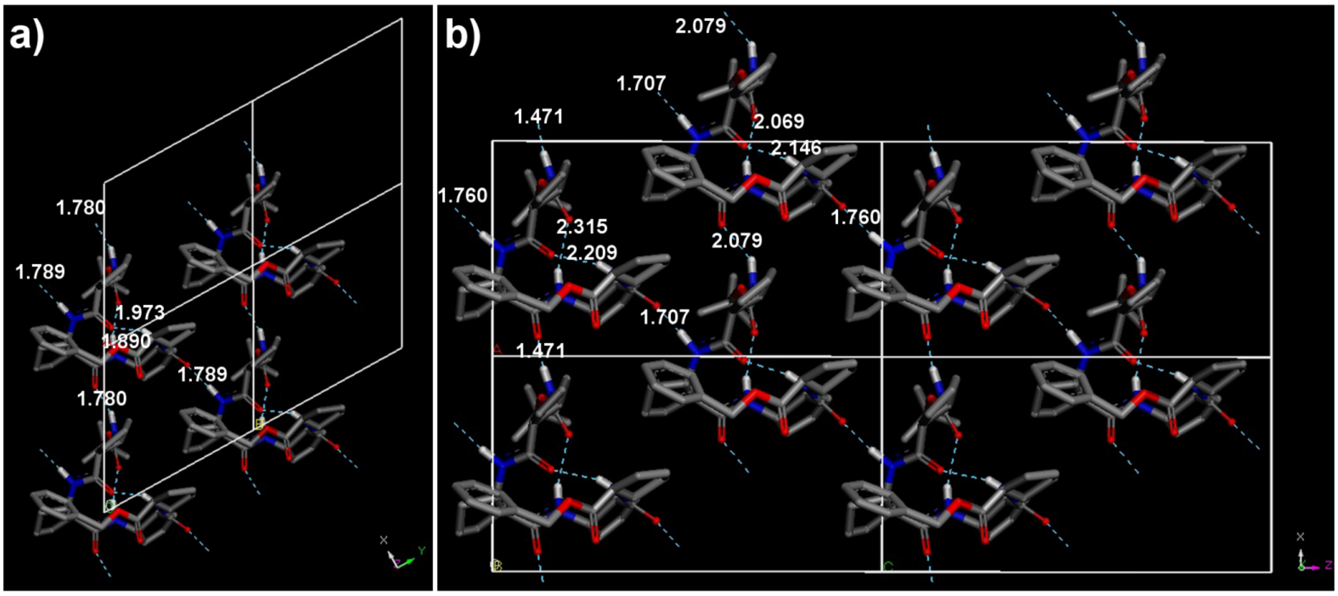
Supporting Figure S1. SEM images of the self-assembled structures of $ACPC_4$ by the self-assembly in solutions of a) methanol/water; b) THF/water; c) THF/P123 aqueous solution (8g/L). Elusive shapes were observed in the conditions of a) and b). Ferule-shape was obtained in the presence of P123 additive, but the homogeneities in shape and size were poorer than those from longer analogues.



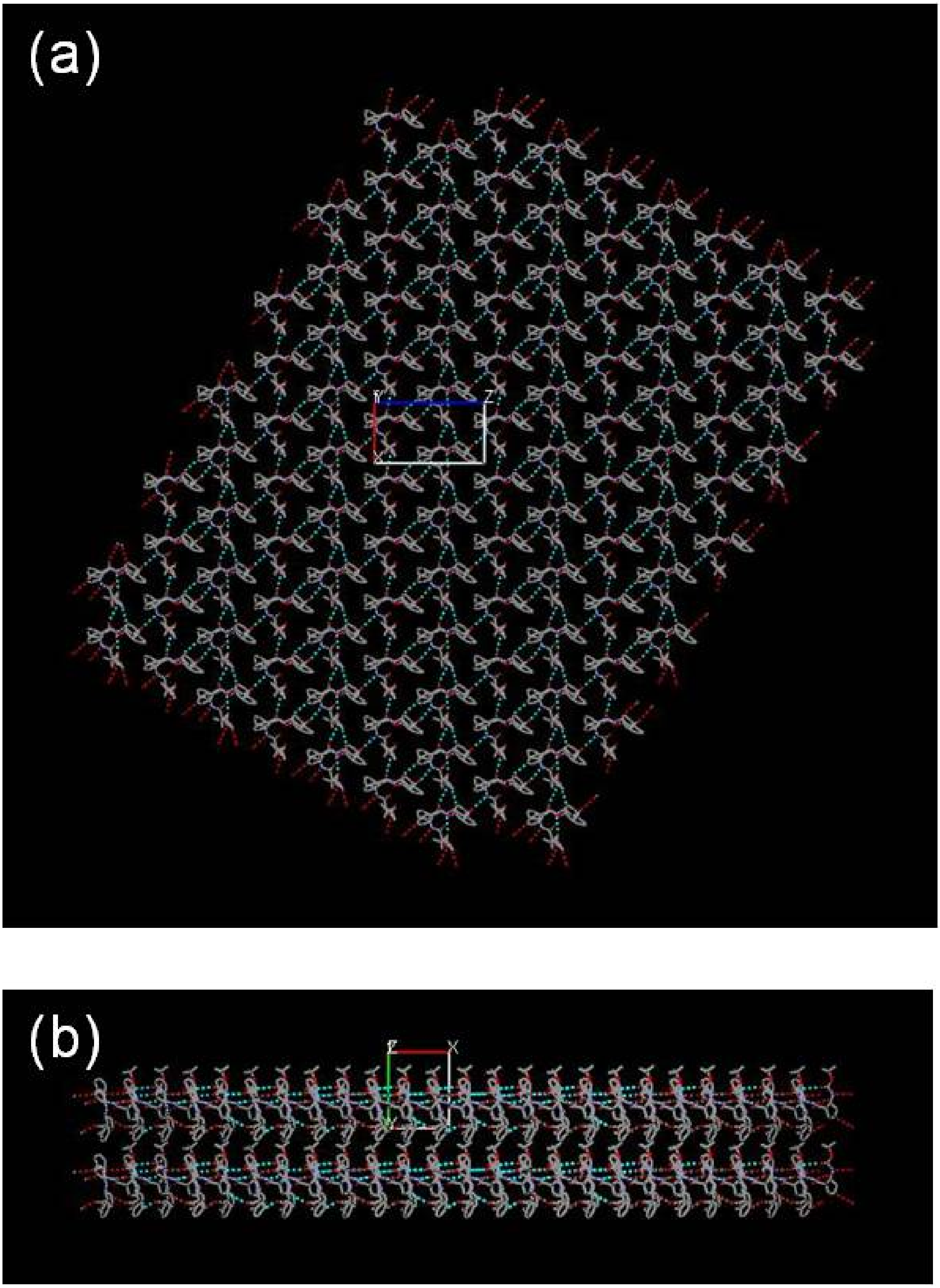
Supporting Figure S2. SEM images of the self-assembled structures of $ACPC_4$ obtained from the evaporation-induced self-assembly of methanol/ water binary solutions with increasing water content a) 0%; b) 10%; c) 20%. Regardless of water content, microtubes with rectangular cross-section were observed, but the best homogeneity in shape and size distribution was obtained from 10% water content.



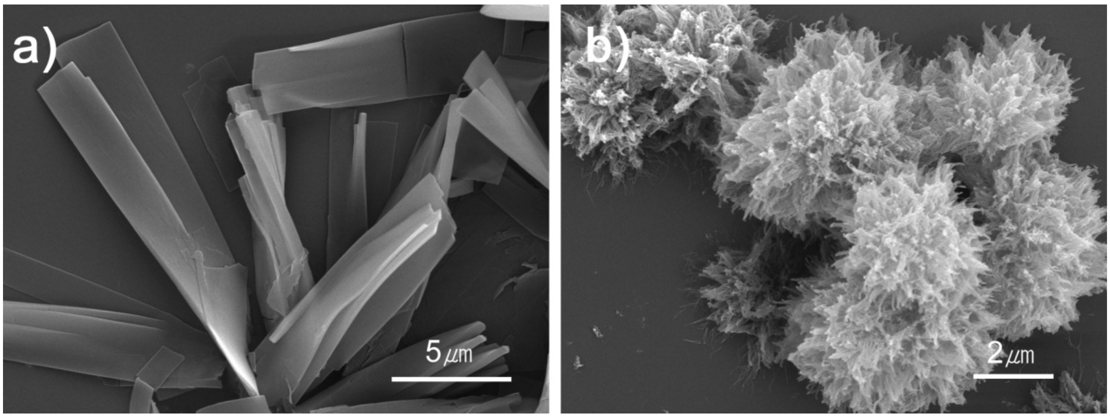
Supporting Figure S3. Molecular structures of (a) $ACPC_4$ single crystal, (b) $ACPC_4$ microtubes in the unit cell. (blue dotted lines represent inter/intra hydrogen bonds.)



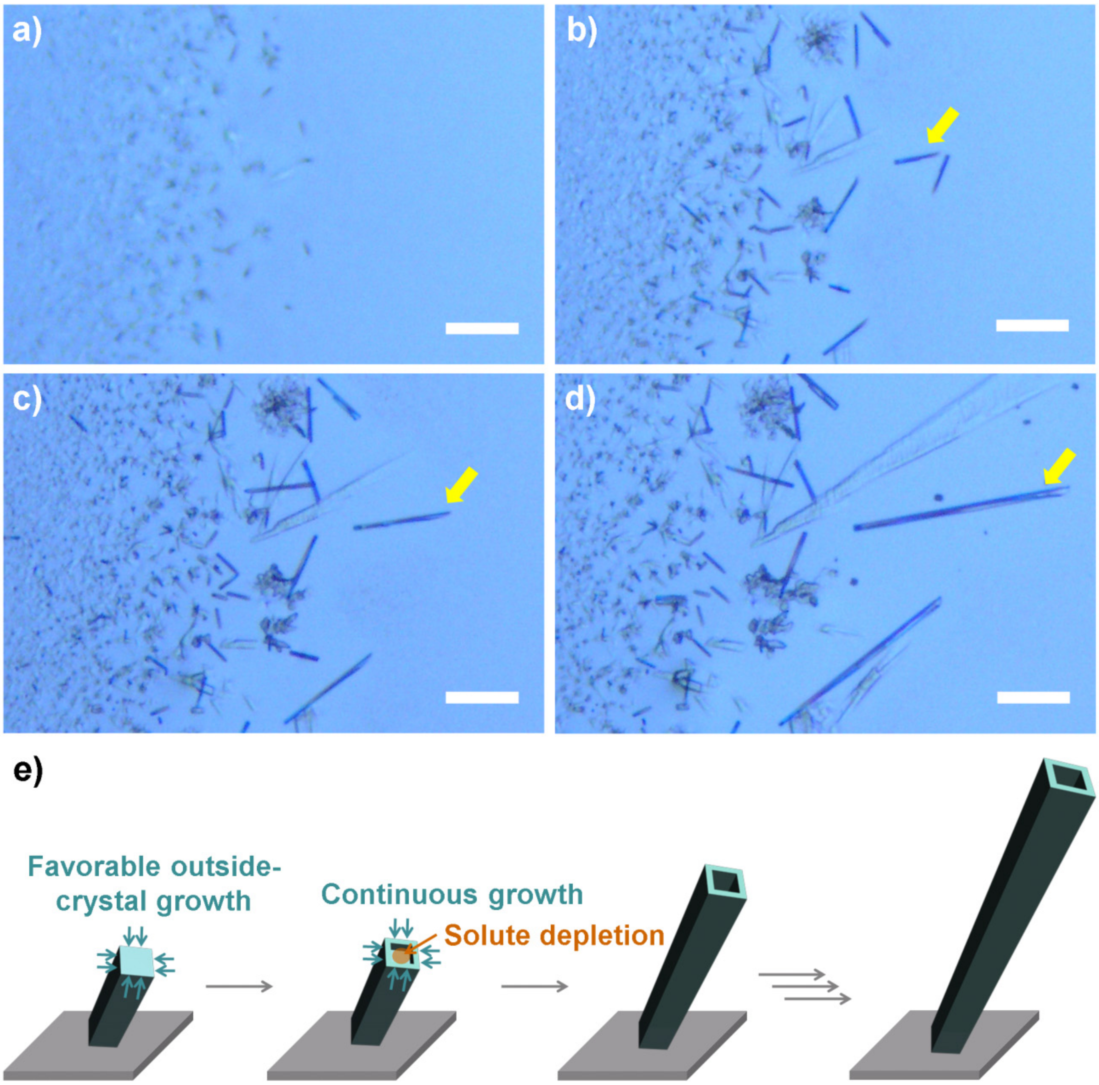
Supporting Figure S4. Molecular structures of (a) $ACPC_4$ single crystal, (b) $ACPC_4$ microtubes in the 2x2 unit cells. The structure was lined along (a) the c and (b) b axis, respectively. (blue dotted lines and numbers represent inter/intra hydrogen bonds and distances, respectively.)



Supporting Figure S5. The molecular network of the $ACPC_4$ microtubes. The structure was lined along (a) the b and (b) c axis, respectively.



Supporting Figure S6. SEM images of self-assembled structures of a) BocNH-*trans*-ACPC$_4$-OH, b) BocNH-*trans*-ACPC$_4$-OMe.



Supporting Figure S7. Optical microscope images of tubular structure growth according to the evaporation times (a) 20s, (b) 60s, (c) 90s, (d) 180s. At initial stage, no morphologies were observed. After 20 sec, tiny nucleates were formed from a circumference (a). As the evaporation proceeded, nucleates grew up into radial bundles and 1D structures (b). Microtube morphologies were developed as the remnant solvent was removed (yellow and red arrows) (c-d). Scale bar: 10 μm. (e) Plausible formation mechanism of microtubes.

Supporting Table S1. Inter-residue NOEs of $ACPC_4$ in pyridine-d_5.

Residue	Proton	Residue	Proton	NOE
1	H_α	2	H_N	strong
1	H_α	3	H_N	strong
1	H_β	2	H_N	medium
1	H_β	3	H_N	medium
1	H_β	4	H_N	weak
1	H_β	3	H_α	medium
1	H_β	3	H_ε	weak-medium
1	CH_3	2	H_α	medium
1	CH_3	3	H_α	weak-medium
1	CH_3	3	H_N	medium
2	H_α	3	H_N	strong
2	H_β	3	H_N	medium
2	H_β	4	H_N	medium
2	H_β	4	H_α	weak-medium
2	H_β	4	H_ε	medium
3	H_α	4	H_N	strong
3	H_α	4	H_β	weak
3	H_β	4	H_N	medium
3	H_β	4	H_α	weak-medium

* The NOEs were classified into four groups of strong, , medium, weak-medium, weak based on intensity. (Strong: 2.6Å, medium: 3.5Å, weak-medium: 4.0Å, weak: 4.5Å)

Supporting Table S2. Atomic Fractional Coordinates, Displacement and Population Parameters for β-Peptide Tetramer (Single Crystal Data)

Atom label	x	y	z	Uiso	Occupancy	multiplicity
C1	0.1835(7)	-0.2457(8)	0.6162(5)	0.0857(16)	1	1
C2	0.3154(8)	-0.3915(9)	0.6119(6)	0.100(2)	1	1
C3	0.3437(8)	-0.4775(8)	0.5154(7)	0.105(2)	1	1
C4	0.2350(10)	-0.4147(9)	0.4271(6)	0.1029(19)	1	1
C5	0.1019(8)	-0.2683(8)	0.4309(5)	0.0876(17)	1	1
C6	0.0720(6)	-0.1801(6)	0.5254(5)	0.0751(13)	1	1
C7	-0.0781(8)	-0.0222(8)	0.5270(7)	0.106(2)	1	1
C8	-0.1539(6)	0.2180(6)	0.6170(5)	0.0724(13)	1	1
C9	-0.0974(5)	0.3286(5)	0.6559(4)	0.0610(11)	1	1
C10	-0.1039(8)	0.4407(8)	0.5555(5)	0.1005(19)	1	1
C11	-0.1619(16)	0.5952(11)	0.6013(8)	0.173(4)	1	1
C12	-0.1878(11)	0.5889(7)	0.7196(6)	0.126(3)	1	1
C13	-0.2028(5)	0.4389(5)	0.7460(4)	0.0718(13)	1	1
C14	-0.2488(5)	0.4390(5)	0.9512(4)	0.0639(12)	1	1
C15	-0.1812(5)	0.3566(5)	1.0661(4)	0.0563(10)	1	1
C16	-0.2492(9)	0.4681(7)	1.1662(5)	0.0976(18)	1	1
C17	-0.3080(19)	0.3911(18)	1.2436(9)	0.239(8)	1	1
C18	-0.3191(8)	0.2681(8)	1.2053(6)	0.114(3)	1	1
C19	-0.2259(5)	0.2230(5)	1.0934(4)	0.0578(11)	1	1
C20	-0.0798(5)	-0.0610(5)	1.0680(4)	0.0558(10)	1	1
C21	0.0833(4)	-0.2104(5)	1.0698(3)	0.0502(9)	1	1
C22	0.0708(9)	-0.3568(7)	1.1145(5)	0.0931(17)	1	1
C23	0.1029(10)	-0.4563(8)	1.0213(6)	0.119(3)	1	1
C24	0.2131(7)	-0.4269(6)	0.9412(5)	0.0758(14)	1	1
C25	0.1478(5)	-0.2486(5)	0.9480(4)	0.0505(9)	1	1
C26	0.2405(4)	-0.0607(4)	0.8785(3)	0.0434(8)	1	1
C27	0.3859(4)	-0.0366(4)	0.8521(3)	0.0449(9)	1	1
C28	0.3941(6)	0.0023(6)	0.7232(4)	0.0649(12)	1	1
C29	0.4289(12)	0.1378(11)	0.7151(5)	0.141(3)	1	1
C30	0.4707(6)	0.1644(6)	0.8295(4)	0.0677(12)	1	1
C31	0.3801(5)	0.1058(5)	0.9108(3)	0.0475(9)	1	1
C32	0.3672(5)	0.0665(5)	1.1175(3)	0.0515(10)	1	1
C33	0.4100(6)	0.0066(6)	1.3256(4)	0.0688(13)	1	1
C34	0.5557(9)	-0.0291(12)	1.4003(6)	0.133(3)	1	1
C35	0.3811(13)	-0.1341(11)	1.3251(7)	0.154(4)	1	1

C36	0.2638(11)	0.1503(11)	1.3613(7)	0.157(4)	1	1
N1	-0.1524(4)	0.3731(4)	0.8616(3)	0.0620(9)	1	1
N2	-0.0804(4)	0.0695(4)	1.1017(3)	0.0514(8)	1	1
N3	0.2741(3)	-0.2048(4)	0.9198(3)	0.0484(8)	1	1
N4	0.4495(4)	0.0710(5)	1.0255(3)	0.0623(10)	1	1
O1	-0.0356(4)	0.0896(4)	0.5729(3)	0.0812(10)	1	1
O2	-0.2910(5)	0.2385(6)	0.6235(7)	0.161(3)	1	1
O3	-0.3834(4)	0.5568(4)	0.9382(3)	0.1022(13)	1	1
O4	-0.2045(4)	-0.0614(5)	1.0337(4)	0.1034(14)	1	1
O5	0.0996(3)	0.0462(3)	0.8594(2)	0.0563(7)	1	1
O6	0.2252(3)	0.0950(4)	1.1167(2)	0.0657(8)	1	1
O7	0.4616(4)	0.0313(5)	1.2127(3)	0.0801(10)	1	1

Supporting Table S3. Atomic Displacement Parameters for β-Peptide Tetramer (Single Crystal Data)

Atom label	U11	U22	U33	U23	U13	U12
C1	0.089(4)	0.112(5)	0.069(3)	-0.012(3)	-0.006(3)	-0.058(4)
C2	0.092(4)	0.114(5)	0.097(5)	0.025(4)	-0.022(4)	-0.054(4)
C3	0.101(5)	0.078(4)	0.126(6)	0.000(4)	0.013(5)	-0.037(4)
C4	0.135(6)	0.093(5)	0.084(4)	-0.018(4)	0.016(4)	-0.056(5)
C5	0.119(5)	0.099(5)	0.066(3)	0.007(3)	-0.026(3)	-0.071(4)
C6	0.081(3)	0.078(3)	0.088(4)	-0.009(3)	-0.003(3)	-0.055(3)
C7	0.088(4)	0.104(5)	0.142(5)	-0.034(4)	-0.011(4)	-0.057(4)
C8	0.052(3)	0.061(3)	0.100(4)	0.007(3)	-0.001(3)	-0.025(2)
C9	0.048(2)	0.058(3)	0.073(3)	0.004(2)	-0.001(2)	-0.023(2)
C10	0.118(5)	0.095(5)	0.094(4)	0.006(4)	0.022(4)	-0.058(4)
C11	0.283(12)	0.115(6)	0.144(8)	-0.017(5)	0.100(8)	-0.112(7)
C12	0.199(8)	0.050(3)	0.100(5)	0.000(3)	0.026(5)	-0.038(4)
C13	0.048(2)	0.054(3)	0.079(3)	0.010(2)	0.001(2)	0.001(2)
C14	0.053(2)	0.048(3)	0.083(3)	0.004(2)	0.011(2)	-0.019(2)
C15	0.046(2)	0.048(2)	0.068(3)	-0.005(2)	0.0087(19)	-0.0168(19)
C16	0.117(5)	0.082(4)	0.088(4)	-0.024(3)	0.013(4)	-0.042(4)
C17	0.413(19)	0.356(17)	0.152(8)	-0.169(10)	0.185(11)	-0.336(17)
C18	0.095(4)	0.083(4)	0.130(5)	0.008(4)	0.063(4)	-0.017(3)
C19	0.039(2)	0.054(3)	0.079(3)	0.004(2)	0.008(2)	-0.0215(19)
C20	0.047(2)	0.071(3)	0.060(3)	-0.017(2)	0.0144(19)	-0.036(2)
C21	0.048(2)	0.050(2)	0.052(2)	-0.0084(18)	0.0019(18)	-0.0236(19)
C22	0.137(5)	0.079(4)	0.080(3)	-0.002(3)	0.012(3)	-0.065(4)
C23	0.173(7)	0.081(4)	0.136(6)	-0.028(4)	0.059(5)	-0.086(5)
C24	0.092(4)	0.058(3)	0.094(4)	-0.022(3)	0.017(3)	-0.048(3)
C25	0.045(2)	0.048(2)	0.058(2)	-0.0106(18)	0.0041(17)	-0.0209(18)
C26	0.040(2)	0.042(2)	0.043(2)	-0.0045(16)	-0.0034(15)	-0.0153(18)
C27	0.0369(18)	0.039(2)	0.050(2)	-0.0004(17)	0.0037(16)	-0.0116(16)
C28	0.070(3)	0.069(3)	0.054(3)	-0.013(2)	0.016(2)	-0.032(2)
C29	0.248(9)	0.222(9)	0.063(4)	0.002(4)	0.010(4)	-0.201(8)
C30	0.083(3)	0.069(3)	0.064(3)	-0.008(2)	0.013(2)	-0.046(3)
C31	0.047(2)	0.050(2)	0.043(2)	-0.0024(17)	0.0018(17)	-0.0220(19)
C32	0.040(2)	0.068(3)	0.053(2)	-0.009(2)	-0.0012(18)	-0.031(2)
C33	0.073(3)	0.097(4)	0.046(3)	-0.005(2)	0.002(2)	-0.048(3)
C34	0.113(5)	0.228(9)	0.071(4)	0.016(5)	-0.019(4)	-0.095(6)
C35	0.267(12)	0.162(8)	0.104(5)	0.021(5)	-0.016(6)	-0.162(9)
C36	0.160(7)	0.152(7)	0.097(5)	-0.058(5)	0.023(5)	-0.020(6)

N1	0.0448(18)	0.048(2)	0.071(2)	0.0037(18)	0.0086(18)	-0.0052(16)
N2	0.0419(17)	0.0487(19)	0.063(2)	-0.0046(16)	-0.0029(15)	-0.0215(15)
N3	0.0343(15)	0.0371(18)	0.067(2)	0.0021(15)	-0.0002(14)	-0.0125(13)
N4	0.0406(17)	0.104(3)	0.051(2)	-0.0122(18)	0.0083(15)	-0.0414(19)
O1	0.065(2)	0.083(2)	0.105(3)	-0.025(2)	0.0061(18)	-0.0420(19)
O2	0.064(3)	0.108(3)	0.317(9)	-0.043(4)	0.022(3)	-0.045(3)
O3	0.056(2)	0.071(2)	0.115(3)	0.016(2)	0.0186(19)	0.0193(17)
O4	0.0437(18)	0.109(3)	0.171(4)	-0.063(3)	0.013(2)	-0.0427(19)
O5	0.0383(14)	0.0446(15)	0.0737(19)	0.0028(13)	-0.0063(12)	-0.0106(13)
O6	0.0433(16)	0.095(2)	0.0639(18)	-0.0084(15)	0.0069(13)	-0.0374(15)
O7	0.0581(18)	0.143(3)	0.0518(19)	0.0017(18)	-0.0013(15)	-0.059(2)

Supporting Table S4. Data Collection and Crystallographic Parameters for $ACPC_4$ in microtubes.

material	β-Peptide Foldamer
unit cell composition	
refined structure	C36 N4 O7 (Z=2)
symmetry	Triclinic
space group	*P*1
a, Å	9.31269(26)
b, Å	11.69486(33)
c, Å	16.9093(6)
α, °	92.945(4))
β, °	90.043(6)
γ, *°*	90.094(6)
cell volume, $Å^3$	1839.17(10)
diffractometer	Rigaku D / MAX-2500, Cu Kα
temperature, °C	room temperature
wave length, Å	1.54178
2θ scan range, °	4 - 70
Δθ, °	0.02
no. observations	3438
no. geometric restraints	102
no. structural parameters	333
R_p, %	4.85
R_{wp}, %	6.57
R_F, %	2.98
Goodness of Fit	2.65

Supporting Table S5. Atomic Coordinates, Displacement and Population Parameters for β-Peptide Tetramer

atom	*x*	*y*	*z*	occupancy	U_{iso}, $10^2 \times Å^2$	multiplicity
			The First Unit of $ACPC_4$			
C1	0.9112(231)	0.9779(176)	0.5127(113)	1	1.10(7)	1
C2	0.9585(30)	0.9659(22)	0.4370(9)	1	1.10(7)	1
C3	0.9487(27)	1.0599(17)	0.3920(12)	1	1.10(7)	1
C4	0.8610(25)	1.1485(17)	0.4147(11)	1	1.10(7)	1
C5	0.7922(27)	1.1508(17)	0.4862(11)	1	1.10(7)	1
C6	0.8127(22)	1.0596(15)	0.5337(14)	1	1.10(7)	1
C7	0.7278(27)	1.0639(23)	0.6140(14)	1	1.10(7)	1
C8	0.7779(27)	0.9800(22)	0.7403(12)	1	1.10(7)	1
C9	0.8900(28)	0.9518(22)	0.7987(12)	1	1.10(7)	1
C10	0.9530(29)	1.0327(20)	0.8536(11)	1	1.10(7)	1
C11	0.9686(28)	0.9854(17)	0.9247(12)	1	1.10(7)	1
C12	0.9474(27)	0.8682(18)	0.9218(14)	1	1.10(7)	1
C13	0.8370(28)	0.8430(22)	0.8457(13)	1	1.10(7)	1
C14	0.7915(27)	0.6335(18)	0.8438(13)	1	1.10(7)	1
C15	0.8202(27)	0.5227(18)	0.8071(12)	1	1.10(7)	1
C16	0.8062(24)	0.4230(18)	0.8646(12)	1	1.10(7)	1
C17	0.7131(23)	0.3499(19)	0.8242(11)	1	1.10(7)	1
C18	0.6462(24)	0.3833(19)	0.7570(11)	1	1.10(7)	1
C19	0.7149(26)	0.4899(20)	0.7307(12)	1	1.10(7)	1
C20	0.7263(25)	0.5153(20)	0.5895(12)	1	1.10(7)	1
C21	0.8060(27)	0.5196(20)	0.5143(13)	1	1.10(7)	1
C22	0.7370(27)	0.4812(19)	0.4429(12)	1	1.10(7)	1
C23	0.7392(27)	0.5633(17)	0.3907(12)	1	1.10(7)	1
C24	0.8581(27)	0.6469(20)	0.4051(14)	1	1.10(7)	1
C25	0.8728(26)	0.6470(19)	0.4952(14)	1	1.10(7)	1
C26	1.0661(25)	0.7065(21)	0.5955(12)	1	1.10(7)	1
C27	1.2096(24)	0.7385(21)	0.6169(12)	1	1.10(7)	1
C28	1.2542(25)	0.8619(20)	0.6375(13)	1	1.10(7)	1
C29	1.3520(27)	0.8584(18)	0.7023(12)	1	1.10(7)	1
C30	1.3922(28)	0.7497(18)	0.7193(13)	1	1.10(7)	1
C31	1.2783(25)	0.6696(18)	0.6858(13)	1	1.10(7)	1
C32	1.2350(22)	0.4580(17)	0.6603(14)	1	1.10(7)	1
C33	1.2514(21)	0.2431(18)	0.6108(11)	1	1.10(7)	1
C34	1.3701(22)	0.1832(20)	0.6202(14)	1	1.10(7)	1

C35	1.1415(22)	0.2180(20)	0.6717(13)	1	1.10(7)	1
C36	1.2077(25)	0.2484(20)	0.5340(11)	1	1.10(7)	1
N37	0.8461(28)	0.7344(17)	0.8163(12)	1	1.10(7)	1
N38	0.7822(23)	0.4822(18)	0.6562(12)	1	1.10(7)	1
N39	1.0140(24)	0.6758(19)	0.5256(12)	1	1.10(7)	1
N40	1.3308(22)	0.5505(17)	0.6713(13)	1	1.10(7)	1
O41	0.8284(23)	1.0270(21)	0.6701(12)	1	1.10(7)	1
O42	0.6476(20)	0.9801(17)	0.7497(11)	1	1.10(7)	1
O43	0.6959(23)	0.6406(18)	0.8987(12)	1	1.10(7)	1
O44	0.6164(20)	0.5438(17)	0.5891(12)	1	1.10(7)	1
O45	0.9848(23)	0.7235(19)	0.6418(11)	1	1.10(7)	1
O46	1.1102(19)	0.4611(16)	0.6707(12)	1	1.10(7)	1
O47	1.3176(20)	0.3576(16)	0.6396(12)	1	1.10(7)	1
			The Second Unit of $ACPC_4$			
C1	0.3564(29)	0.9848(26)	0.0210(13)	1	4.40(10)	1
C2	0.4099(31)	0.9770(22)	-0.0536(11)	1	4.40(10)	1
C3	0.3976(27)	1.0728(17)	-0.0947(12)	1	4.40(10)	1
C4	0.3249(25)	1.1633(18)	-0.0616(11)	1	4.40(10)	1
C5	0.2700(25)	1.1628(17)	0.0125(11)	1	4.40(10)	1
C6	0.2807(26)	1.0698(17)	0.0585(13)	1	4.40(10)	1
C7	0.2187(27)	1.0735(22)	0.1404(14)	1	4.40(10)	1
C8	0.2824(24)	0.9715(23)	0.2556(11)	1	4.40(10)	1
C9	0.3862(25)	0.9564(22)	0.3110(11)	1	4.40(10)	1
C10	0.4467(27)	1.0353(21)	0.3712(11)	1	4.40(10)	1
C11	0.4602(26)	0.9884(17)	0.4434(12)	1	4.40(10)	1
C12	0.4420(26)	0.8696(18)	0.4413(14)	1	4.40(10)	1
C13	0.3420(28)	0.8400(22)	0.3616(13)	1	4.40(10)	1
C14	0.3116(28)	0.6289(16)	0.3579(12)	1	4.40(10)	1
C15	0.3369(28)	0.5279(17)	0.3184(12)	1	4.40(10)	1
C16	0.3350(24)	0.4163(18)	0.3701(12)	1	4.40(10)	1
C17	0.2418(23)	0.3446(19)	0.3323(11)	1	4.40(10)	1
C18	0.1564(24)	0.3774(20)	0.2732(12)	1	4.40(10)	1
C19	0.2163(26)	0.4945(20)	0.2498(12)	1	4.40(10)	1
C20	0.2118(25)	0.5272(20)	0.1059(12)	1	4.40(10)	1
C21	0.2834(26)	0.5259(21)	0.0263(13)	1	4.40(10)	1
C22	0.1975(26)	0.4932(18)	-0.0411(13)	1	4.40(10)	1
C23	0.1812(25)	0.5792(18)	-0.0859(13)	1	4.40(10)	1
C24	0.3092(28)	0.6550(20)	-0.0824(14)	1	4.40(10)	1

C25	0.3441(25)	0.6488(20)	0.0062(14)	1	4.40(10)	1
C26	0.5428(25)	0.7111(22)	0.0927(12)	1	4.40(10)	1
C27	0.6886(24)	0.7452(22)	0.1067(13)	1	4.40(10)	1
C28	0.7347(26)	0.8792(21)	0.1198(13)	1	4.40(10)	1
C29	0.8434(27)	0.8851(18)	0.1769(13)	1	4.40(10)	1
C30	0.8972(28)	0.7766(19)	0.1907(13)	1	4.40(10)	1
C31	0.7714(26)	0.6917(19)	0.1708(13)	1	4.40(10)	1
C32	0.7403(22)	0.4781(18)	0.1605(14)	1	4.40(10)	1
C33	0.7353(23)	0.2596(19)	0.1208(11)	1	4.40(10)	1
C34	0.8528(27)	0.1847(21)	0.0930(14)	1	4.40(10)	1
C35	0.6184(26)	0.2675(21)	0.0591(14)	1	4.40(10)	1
C36	0.6922(24)	0.2312(20)	0.1935(11)	1	4.40(10)	1
N37	0.3624(27)	0.7342(17)	0.3296(12)	1	4.40(10)	1
N38	0.2791(24)	0.4926(19)	0.1712(12)	1	4.40(10)	1
N39	0.4923(24)	0.6746(19)	0.0248(13)	1	4.40(10)	1
N40	0.8252(22)	0.5763(17)	0.1555(13)	1	4.40(10)	1
O41	0.3223(23)	1.0142(21)	0.1932(11)	1	4.40(10)	1
O42	0.1440(21)	0.9696(18)	0.2617(10)	1	4.40(10)	1
O43	0.2362(25)	0.6225(19)	0.4208(13)	1	4.40(10)	1
O44	0.0929(21)	0.5608(18)	0.1171(12)	1	4.40(10)	1
O45	0.4752(23)	0.7376(20)	0.1476(11)	1	4.40(10)	1
O46	0.6332(20)	0.4854(17)	0.1924(12)	1	4.40(10)	1
O47	0.8043(20)	0.3765(16)	0.1273(12)	1	4.40(10)	1

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