Electronic Supplementary Material (ESI) for Soft Matter.

Supporting Information for:

Influence of Central Sidechain on Self-Assembly of Glycine-X-Glycine Peptides

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Figures

Figure S1. Representative decompositions of the first and last spectra measured at the beginning and end of the kinetic experiments for GFG at pH 3.4, respectively. The band position monitored was 1633 cm^{-1}. The fractional intensities of the band with respect to the amide I' region were plotted as a function of time. The resultant plot was fitted with an exponential and is presented in Table 2.

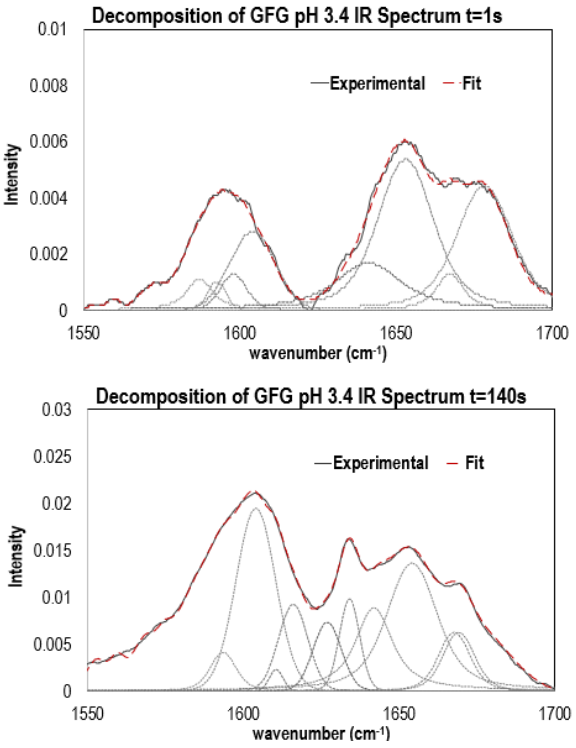

Figure S2. XRD raw data (black dots), Rietveld refinement (red line), the difference between raw and calculated data (blue line), and Bragg reflections (vertical magenta lines) of a) GDG, b) GHG, c) GFG, d) GYG and e) GAG pure peptides.

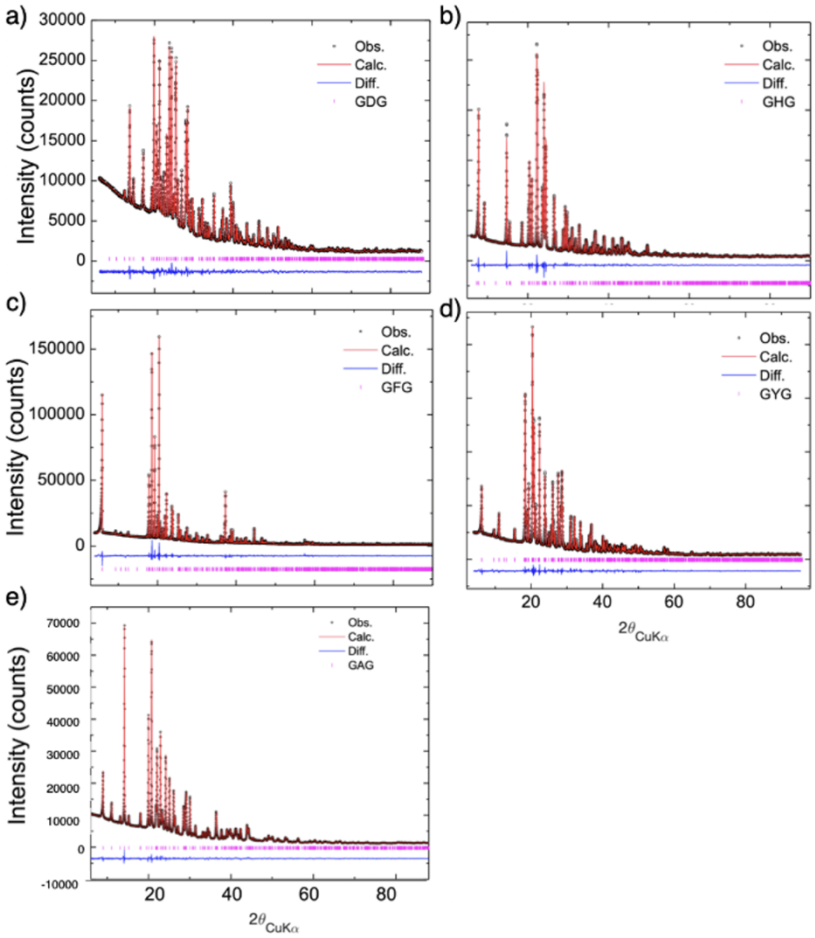

Figure S3: Direct comparison between the raw diffractograms of powder and almost dried gels for each peptide, a) GAG, b) GDG, c) GFG, d) GHG, e) GWG and f) GYG.

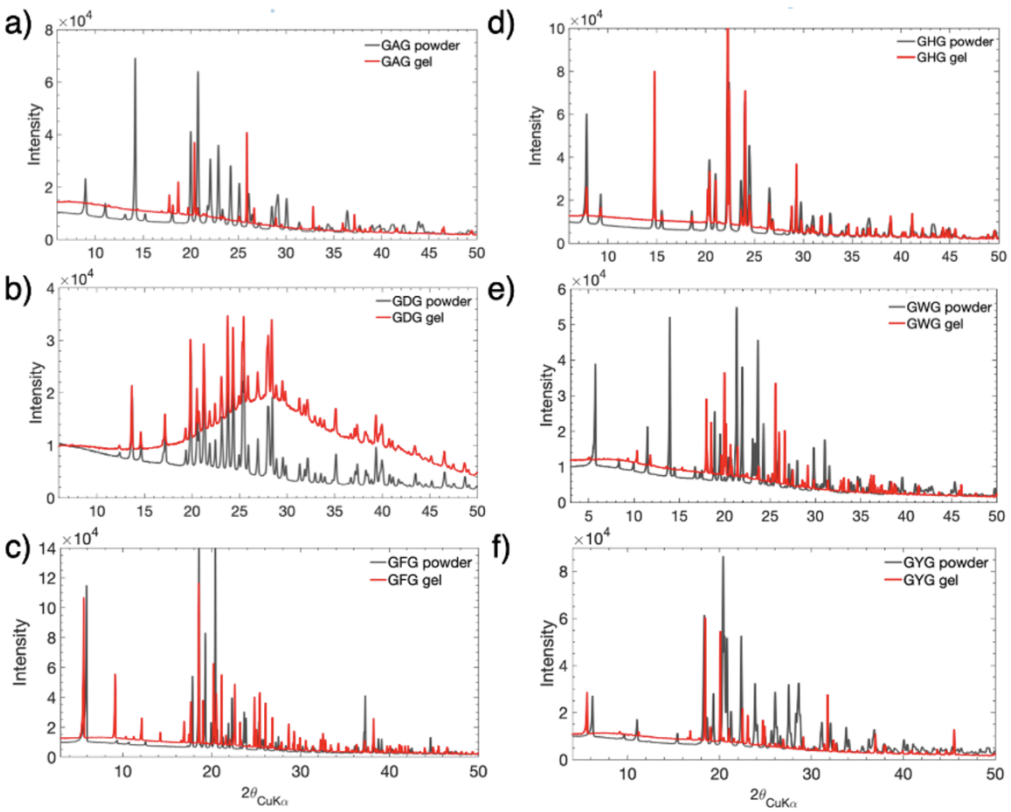

Table S1. GAG Fractional Atom Coordinates.

Atom	x	y	z
C1	0.5597(7)	0.4801(5)	0.4218(14)
N2	0.5773(4)	0.4194(3)	0.2458(12)
C3	0.5438(5)	0.5671(4)	0.3011(15)
O4	0.5577(4)	0.4687(3)	0.6778(8)
C5	0.5950(5)	0.3347(4)	0.3419(14)
N6	0.4552(5)	0.6113(3)	0.4325(10)

C7	0.6483(4)	0.6184(4)	0.3232(12)
C8	0.5058(6)	0.2982(5)	0.5207(17)
C9	0.3558(6)	0.5971(5)	0.3676(15)
O10	0.5293(4)	0.2448(3)	0.6931(11)
O11	0.4139(4)	0.3193(3)	0.4637(10)
O12	0.3274(3)	0.5460(4)	0.1921(8)
C13	0.2751(4)	0.6434(5)	0.5479(14)
N14	0.1659(3)	0.6180(3)	0.4747(9)
H1	0.2806(4)	0.7017(5)	0.5019(14)
H2	0.2905(4)	0.6356(5)	0.7443(14)
H3	0.7031(4)	0.5912(4)	0.2148(12)
H4	0.6341(4)	0.6725(4)	0.2444(12)
H5	0.6722(4)	0.6246(4)	0.5144(12)
H6	0.1603(3)	0.5653(3)	0.5168(9)
H7	0.1211(3)	0.6467(3)	0.5763(9)
H8	0.5773(4)	0.4293(3)	0.0656(12)
H10	0.6592(5)	0.3346(4)	0.4538(14)
H11	0.6051(5)	0.2995(4)	0.1802(14)

H12	0.5247(5)	0.5597(4)	0.1068(15)
H13	0.4695(5)	0.6483(3)	0.5619(10)
H14	0.1513(3)	0.6252(3)	0.2971(9)

Table S2. GAG bond lengths.

Atom 1	**Atom 2**	**Bond Length (Å)**
C1	N2	1.300(10)
C3	C1	1.519(11)
O4	C1	1.229(8)
C5	N2	1.447(9)
C3	N6	1.453(9)
C7	C3	1.545(8)
C5	C8	1.517(10)
C9	N6	1.298(10)
O10	C8	1.219(9)
O11	C8	1.226(9)
O12	C9	1.220(9)
C13	C9	1.515(10)

C13	N14	1.464(7)

Table S3. GAG bond angles.

Atom 1	Atom 2	Atom 3	Bond Angle (°)
C3	C1	N2	117.713(59)
O4	C1	N2	121.851(72)
O4	C1	C3	120.424(69)
C5	N2	C1	121.562(60)
C1	C3	N6	112.577(56)
C7	C3	C1	110.569(53)
C7	C3	N6	110.776(54)
C8	C5	N2	115.146(51)
C3	N6	C9	122.697(56)
O10	C8	C5	117.955(63)
O11	C8	C5	117.216(64)
O11	C8	O10	124.497(69)
O12	C9	N6	123.846(69)
C13	C9	N6	114.568(58)

O12	C9	C13	121.343(66)
C9	C13	N14	110.437(60)

Table S4. GAG Torsion Angle Data

Atom 1	**Atom 2**	**Atom 3**	**Atom 4**	**Torsion Angle (°)**
C3	C1	N2	C5	179.038
O4	C1	N2	C5	0.335
N6	C3	C1	N2	136.15
C7	C3	C1	N2	-99.355
O4	C1	C3	N6	-45.127
O4	C1	C3	C7	79.368
C8	C5	N2	C1	57.182
C1	C3	N6	C9	-78.604
C7	C3	N6	C9	157.015
O10	C8	C5	N2	-151.969
O11	C8	C5	N2	34.34
O12	C9	N6	C3	-0.072

C13	C9	N6	C3	174.309
N6	C9	C13	N14	-175.215
O12	C9	C13	N14	-0.679

Table S5. Hydrogen-bonding Interaction Analysis for GAG.

Donor	**Acceptor**	**D-H (Å)**	**H...A (Å)**	**D...A (Å)**	**D-H...A (°)**	**Type**
N2-H8	O4	0.87	1.961	2.819	169.0	intermolecular
N6-H13	O10	0.87	1.933	2.785	165.5	intermolecular
N14-H6	O12	0.87	1.972	2.821	165.2	intermolecular
N14-H7	O11	0.87	1.966	2.717	143.8	intermolecular
N14-H14	O11	0.87	1.989	2.807	156.3	intermolecular

Table S6. GDG Fractional Atom Coordinates.

Atom	x	y	z
C1	0.3676(5)	0.2532(5)	0.0594(18)
C2	0.2995(4)	0.3070(6)	-0.083(2)
C3	0.4376(4)	0.3295(5)	0.0831(15)
N4	0.3910(4)	0.1624(4)	-0.1012(11)
N5	0.2520(4)	0.3579(5)	0.0796(17)
O6	0.2959(3)	0.3148(4)	-0.3411(10)
C7	0.5070(4)	0.2864(6)	0.2372(17)
C8	0.3560(5)	0.0735(6)	-0.0739(17)
C9	0.1873(4)	0.4174(6)	-0.0292(19)
O10	0.4919(3)	0.2150(3)	0.4221(9)
O11	0.5735(3)	0.3169(3)	0.1991(10)
C12	0.3874(4)	-0.0116(5)	-0.2632(15)
O13	0.3075(3)	0.0552(3)	0.1078(12)
C14	0.1136(5)	0.4054(6)	0.145(2)
N15	0.3469(3)	-0.1092(3)	-0.2068(11)
O16	0.1135(3)	0.3401(4)	0.3313(11)
O17	0.0582(3)	0.4620(3)	0.0961(9)

H1	0.3525(5)	0.2326(5)	0.2402(18)
H2	0.1760(4)	0.3960(6)	-0.2143(19)
H3	0.2009(4)	0.4899(6)	-0.0254(19)
H4	0.4291(4)	0.1701(4)	-0.2291(11)
H5	0.5364(3)	0.1856(3)	0.5335(9)
H6	0.2601(4)	0.3566(5)	0.2616(17)
H7	0.2969(3)	-0.1000(3)	-0.2391(11)
H8	0.3643(3)	-0.1579(3)	-0.3134(11)
H9	0.4428(4)	-0.0232(5)	-0.2245(15)
H10	0.3813(4)	0.0063(5)	-0.4552(15)
H11	0.4195(4)	0.3918(5)	0.1791(15)
H12	0.4539(4)	0.3501(5)	-0.1048(15)
H13	0.3526(3)	-0.1267(3)	-0.0300(11)

Table S7. GDG Bond length data

Atom 1	**Atom 2**	**Bond Length (Å)**
C1	C2	1.517
C3	C1	1.556

C1	N4	1.455
C2	N5	1.301
O6	C2	1.233
C3	C7	1.503
C8	N4	1.301
C9	N5	1.444
O10	C7	1.3
O11	C7	1.219
C12	C8	1.519
O13	C8	1.222
C9	C14	1.518
C12	N15	1.463
O16	C14	1.223
O17	C14	1.22

Table S8. GDG bond angles.

Atom 1	**Atom 2**	**Atom 3**	**Bond Angle (°)**
C3	C1	C2	109.573

C2	C1	N4	110.249
C3	C1	N4	109.617
C1	C2	N5	116.532
O6	C2	C1	121.347
O6	C2	N5	121.289
C1	C3	C7	114.228
C1	N4	C8	122.078
C9	N5	C2	122.382
O10	C7	C3	115.785
O11	C7	C3	123.157
O10	C7	O11	121.039
C12	C8	N4	114.559
O13	C8	N4	123.664
O13	C8	C12	121.347
C14	C9	N5	112.844
C8	C12	N15	110.262
O16	C14	C9	117.84
O17	C14	C9	118.792

O16	C14	O17	123.357

Table S9. GDG Torsion Angle Data

Atom 1	**Atom 2**	**Atom 3**	**Atom 4**	**Torsion Angle (°)**
C3	C1	C2	N5	-87.923
O6	C2	C1	C3	81.761
N4	C1	C2	N5	151.349
O6	C2	C1	N4	-38.967
C2	C1	C3	C7	176.47
C7	C3	C1	N4	-62.419
C2	C1	N4	C8	-83.521
C3	C1	N4	C8	155.777
C1	C2	N5	C9	176.487
O6	C2	N5	C9	6.796
O10	C7	C3	C1	-26.987
O11	C7	C3	C1	154.592

C12	C8	N4	C1	178.77
O13	C8	N4	C1	-8.671
C14	C9	N5	C2	138.767
N4	C8	C12	N15	177.245
O13	C8	C12	N15	4.496
O16	C14	C9	N5	-8.272
O17	C14	C9	N5	170.542

Table S10. Hydrogen-bonding Interaction Analysis for GDG.

Donor	**Acceptor**	**D-H (Å)**	**H...A (Å)**	**D...A (Å)**	**D-H...A (°)**	**Type**
N4-H4	O10	0.90	2.060	2.930	163.0	intermolecular
N5-H6	O6	0.88	2.058	2.909	163.4	intermolecular
O10-H5	O16	1.00	1.506	2.494	167.3	intermolecular
O10-H5	O17	1.00	2.621	3.429	137.6	intermole

						cular
N15-H7	O13	0.88	2.015	2.873	165.3	intermole cular
N15-H8	O16	0.86	2.480	3.062	125.6	intermole cular
N15-H8	O11	0.86	2.146	2.872	141.8	intermole cular
N15-H13	O11	0.88	2.147	2.932	148.9	intermole cular

Table S11. GHG Fractional Atom Coordinates.

Atom	**x**	**y**	**z**
O1	0.0646(5)	-0.0117(10)	0.0405(4)
H2	0.1483(5)	-0.0078(10)	0.0451(4)
H3	0.0244(5)	0.1641(10)	0.0061(4)
C4	0.55980(12)	0.8830(3)	0.32354(13)
C5	0.66282(13)	0.7303(4)	0.29138(12)
O6	0.5543(2)	1.1437(4)	0.3300(3)

N7	0.48300(12)	0.7138(3)	0.35354(13)
N8	0.69293(18)	0.8851(5)	0.19962(13)
C9	0.77145(14)	0.6818(2)	0.39277(6)
C10	0.37850(12)	0.8227(3)	0.38104(13)
C11	0.64634(18)	0.8255(3)	0.09183(11)
C12	0.87510(11)	0.57519(14)	0.35647(4)
C13	0.30570(12)	1.0146(3)	0.29044(13)
O14	0.5898(3)	0.6075(5)	0.0609(2)
C15	0.7003(2)	1.0046(7)	0.01463(14)
N16	0.86339(13)	0.32190(15)	0.29197(5)
C17	0.98457(13)	0.6701(2)	0.37121(6)
O18	0.30111(12)	0.9349(3)	0.19313(13)
O19	0.2545(3)	1.2192(5)	0.3159(2)
N20	0.6326(4)	0.9728(10)	-0.10336(18)
C21	0.96775(14)	0.2711(2)	0.26968(6)
N22	1.04376(14)	0.4829(2)	0.31769(6)
H23	0.5586(4)	0.9865(10)	-0.11774(18)
H24	0.6732(4)	1.0181(10)	-0.14944(18)

H25	0.73599(18)	1.0268(5)	0.21380(13)
H26	0.7819(2)	0.9443(7)	0.02142(14)
H27	0.6977(2)	1.1909(7)	0.02912(14)
H28	0.63341(13)	0.5387(4)	0.26545(12)
H29	0.49180(12)	0.5319(3)	0.34734(13)
H30	0.40250(12)	0.9289(3)	0.44914(13)
H31	0.33010(12)	0.6658(3)	0.39134(13)
H32	1.01332(13)	0.8500(2)	0.40427(6)
H33	0.6357(4)	0.7791(10)	-0.11244(18)
H34	1.11920(14)	0.5127(2)	0.31312(6)
H35	0.75480(14)	0.5655(2)	0.44575(6)
H36	0.79610(14)	0.8713(2)	0.42365(6)
H37	0.99235(14)	0.1159(2)	0.23232(6)

Table S12. GHG Bond length data.

Atom 1	**Atom 2**	**Bond Length (Å)**
C5	C4	1.543
O6	C4	1.234

C4	N7	1.325
C5	N8	1.47
C9	C5	1.558
C10	N7	1.446
C11	N8	1.338
C9	C12	1.487
C10	C13	1.521
O14	C11	1.229
C15	C11	1.53
C12	N16	1.424
C17	C12	1.325
O18	C13	1.253
O19	C13	1.219
C15	N20	1.482
C21	N16	1.342
C17	N22	1.392
C21	N22	1.367

Table S13. GHG Bond angle data.

Atom 1	Atom 2	Atom 3	Bond Angle (°)
O6	C4	C5	122.586
C5	C4	N7	115.121
O6	C4	N7	122.026
C4	C5	N8	109.194
C9	C5	C4	112.903
C9	C5	N8	112.932
C10	N7	C4	121.969
C5	N8	C11	123.59
C5	C9	C12	111.397
C13	C10	N7	112.531
O14	C11	N8	122.396
C15	C11	N8	112.501
O14	C11	C15	122.794
C9	C12	N16	119.073
C9	C12	C17	132.867
C17	C12	N16	108.059
O18	C13	C10	114.266

O19	C13	C10	119.845
O18	C13	O19	125.826
C11	C15	N20	111.163
C21	N16	C12	107.739
C12	C17	N22	107.648
N22	C21	N16	107.742
C17	N22	C21	108.811

Table S14. GHG Torsion angle data.

Atom 1	**Atom 2**	**Atom 3**	**Atom 4**	**Torsion Angle (°)**
O6	C4	C5	N8	-41.73
O6	C4	C5	C9	84.779
N8	C5	C4	N7	144.092
C9	C5	C4	N7	-89.398
C5	C4	N7	C10	-177.029
O6	C4	N7	C10	8.757
C4	C5	N8	C11	-92.222

C9	C5	N8	C11	141.286
C4	C5	C9	C12	-171.295
C12	C9	C5	N8	-46.804
C13	C10	N7	C4	52.51
O14	C11	N8	C5	-12.464
C15	C11	N8	C5	-175.63
C5	C9	C12	N16	-56.552
C17	C12	C9	C5	123.117
O18	C13	C10	N7	38.076
O19	C13	C10	N7	-144.641
N8	C11	C15	N20	-169.589
O14	C11	C15	N20	27.323

Table S15. Hydrogen-bonding Interaction Analysis for GHG.

Donor	**Acceptor**	**D-H (Å)**	**H...A (Å)**	**D...A (Å)**	**D-H...A (°)**	**Type**
O1-H2	O18	0.97	2.225	2.935	129.3	intermolecular

O1-H3	O1	0.99	1.856	2.840	170.6	intermole cular
N7-H29	O6	0.87	2.002	2.850	164.9	intermole cular
N8-H25	N16	0.83	2.086	2.890	163.7	intermole cular
N20-H23	O14	0.84	2.115	2.858	147.1	intermole cular
N20-H24	O18	0.86	2.080	2.652	123.4	intermole cular
N20-H33	O18	0.92	2.136	2.952	147.0	intermole cular
N22-H34	O19	0.91	2.096	2.768	129.7	intermole cular

Table S16. GYG Fractional Atom Coordinates.

Atom	**x**	**y**	**z**
C1	0.5705(2)	0.23894(10)	0.39168(4)

C2	0.47013(17)	0.09544(9)	0.38896(7)
N3	0.4555(2)	0.30450(14)	0.43328(4)
C4	0.4890(3)	0.32321(13)	0.34722(4)
O5	0.2281(3)	0.07057(19)	0.39585(11)
N6	0.6460(2)	-0.00397(11)	0.38068(7)
C7	0.59860(17)	0.38526(14)	0.46075(4)
C8	0.6246(2)	0.27012(11)	0.30434(3)
C9	0.5639(4)	-0.13818(11)	0.36783(4)
O10	0.8477(3)	0.3900(2)	0.46015(7)
C11	0.4373(3)	0.46271(13)	0.49791(6)
C12	0.8401(3)	0.34499(14)	0.28356(4)
C13	0.5074(3)	0.16048(14)	0.27870(4)
C14	0.5155(3)	-0.23720(10)	0.40886(3)
N15	0.5818(5)	0.58781(15)	0.51293(10)
C16	0.9461(3)	0.30697(13)	0.23980(4)
C17	0.6090(3)	0.12434(15)	0.23428(4)
O18	0.4031(6)	-0.34882(15)	0.40198(6)
O19	0.6139(6)	-0.20419(19)	0.44682(5)

C20	0.8432(2)	0.19051(12)	0.21662(3)
O21	0.9401(5)	0.1610(2)	0.17286(5)
H1	0.7635(2)	0.23996(10)	0.39591(4)
H2	0.8147(2)	0.01529(11)	0.38069(7)
H3	1.0934(3)	0.35683(13)	0.22631(4)
H4	0.6073(5)	0.64360(15)	0.48869(10)
H5	0.4827(5)	0.63650(15)	0.53349(10)
H6	0.7351(5)	0.56840(15)	0.52529(10)
H7	0.4015(3)	0.40795(13)	0.52561(6)
H8	0.2606(3)	0.49085(13)	0.48511(6)
H9	0.2831(2)	0.29227(14)	0.43925(4)
H10	0.9176(3)	0.42376(14)	0.29990(4)
H11	0.5024(3)	0.06161(15)	0.21547(4)
H12	0.3832(3)	0.09861(14)	0.29522(4)
H13	0.8237(5)	0.1619(2)	0.14441(5)
H14	0.5356(3)	0.41984(13)	0.35291(4)
H15	0.2914(3)	0.31814(13)	0.34441(4)
H16	0.6818(4)	-0.17501(11)	0.34628(4)

H17	0.3778(4)	-0.12821(11)	0.35268(4)

Tables S17. GYG Bond length data.

Atom 1	Atom 2	Bond Length (Å)
C1	C2	1.475
C1	N3	1.459
C4	C1	1.56
O5	C2	1.225
C2	N6	1.313
C7	N3	1.31
C4	C8	1.484
C9	N6	1.408
O10	C7	1.221
C11	C7	1.52
C12	C8	1.411
C13	C8	1.411
C9	C14	1.532
C11	N15	1.466

C16	C12	1.402
C17	C13	1.406
O18	C14	1.228
O19	C14	1.228
C16	C20	1.401
C17	C20	1.407
O21	C20	1.366

Tables S18. GYG Bond angle data.

Atom 1	**Atom 2**	**Atom 3**	**Bond Angle (°)**
C2	C1	N3	108.883
C4	C1	C2	111.354
C4	C1	N3	109.61
O5	C2	C1	119.917
C1	C2	N6	118.748
O5	C2	N6	121.295
C1	N3	C7	122.676
C8	C4	C1	112.032

C9	N6	C2	122.389
O10	C7	N3	123.258
C11	C7	N3	115.709
O10	C7	C11	120.694
C4	C8	C12	120.226
C4	C8	C13	120.402
C13	C8	C12	118.199
C14	C9	N6	114.977
C7	C11	N15	111.127
C16	C12	C8	121.11
C17	C13	C8	120.715
O18	C14	C9	119.836
O19	C14	C9	116.805
O18	C14	O19	123.074
C12	C16	C20	119.926
C13	C17	C20	119.878
C17	C20	C16	119.364
O21	C20	C16	118.362

O21	C20	C17	121.025

Tables S19. GYG Torsion angle data.

Atom 1	**Atom 2**	**Atom 3**	**Atom 4**	**Torsion Angle (°)**
O5	C2	C1	N3	45.007
N3	C1	C2	N6	-132.712
O5	C2	C1	C4	-75.963
C4	C1	C2	N6	106.318
C2	C1	N3	C7	138.508
C4	C1	N3	C7	-99.459
C2	C1	C4	C8	-65.581
C8	C4	C1	N3	173.875
C1	C2	N6	C9	-166.358
O5	C2	N6	C9	15.956
O10	C7	N3	C1	-15.957
C11	C7	N3	C1	170.697
C12	C8	C4	C1	-106.703

C13	C8	C4	C1	85.895
C14	C9	N6	C2	-89.501
N3	C7	C11	N15	-156.239
O10	C7	C11	N15	30.231
O18	C14	C9	N6	168.568
O19	C14	C9	N6	-17.381

Table S20. Hydrogen-bonding Interaction Analysis for GYG.

Donor	**Acceptor**	**D-H (Å)**	**H...A (Å)**	**D...A (Å)**	**D-H...A (°)**	**Type**
N3-H9	O10	0.87	2.407	3.183	148.8	intermolecular
N6-H2	O5	0.85	2.138	2.972	168.2	intermolecular
N15-H4	O18	0.89	2.670	3.342	133.4	intermolecular
N15-H4	O19	0.89	1.897	2.763	165.2	intermolecular

N15-H5	O19	0.90	2.001	2.799	147.7	intermole cular
N15-H6	O19	0.85	2.408	3.062	134.1	intermole cular
O21-H13	O18	0.99	1.731	2.719	173.7	intermole cular