Powder X-ray diffraction data for all compounds were collected on a Philips powder diffractometer using CuK_{α}-radiation, graphite monochromator on diffracted beam and operating at 40 kV, 30 mA at 293 K.

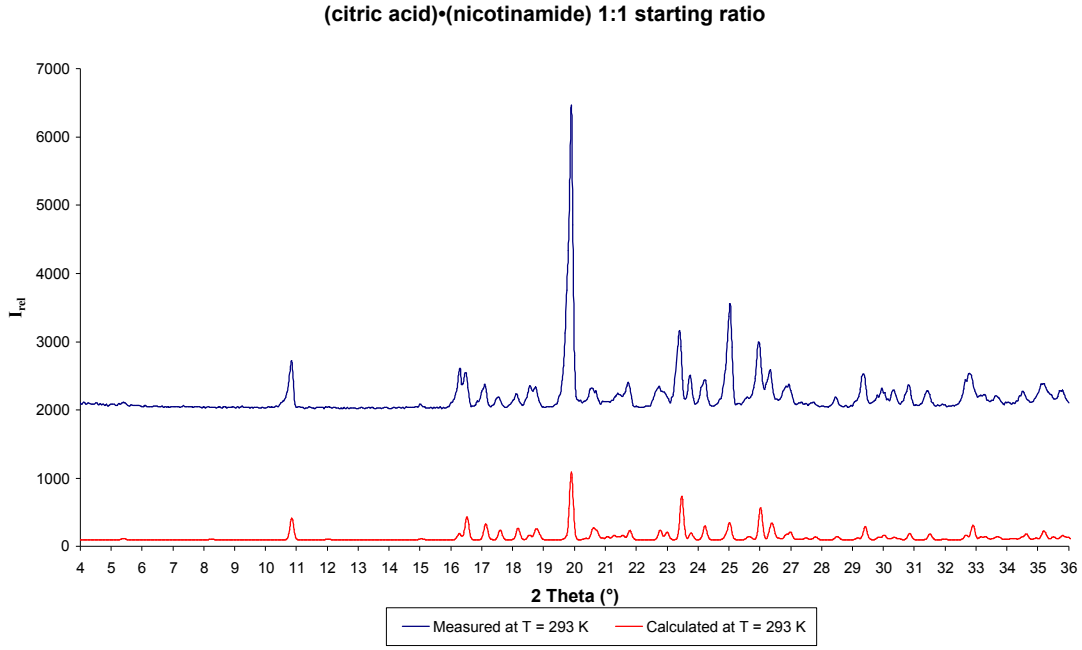

Figure S1: Comparison of powder pattern obtained from co-crystallizing citric acid and nicotinamide in a 1:1 ratio, and that calculated from the single crystal structure.

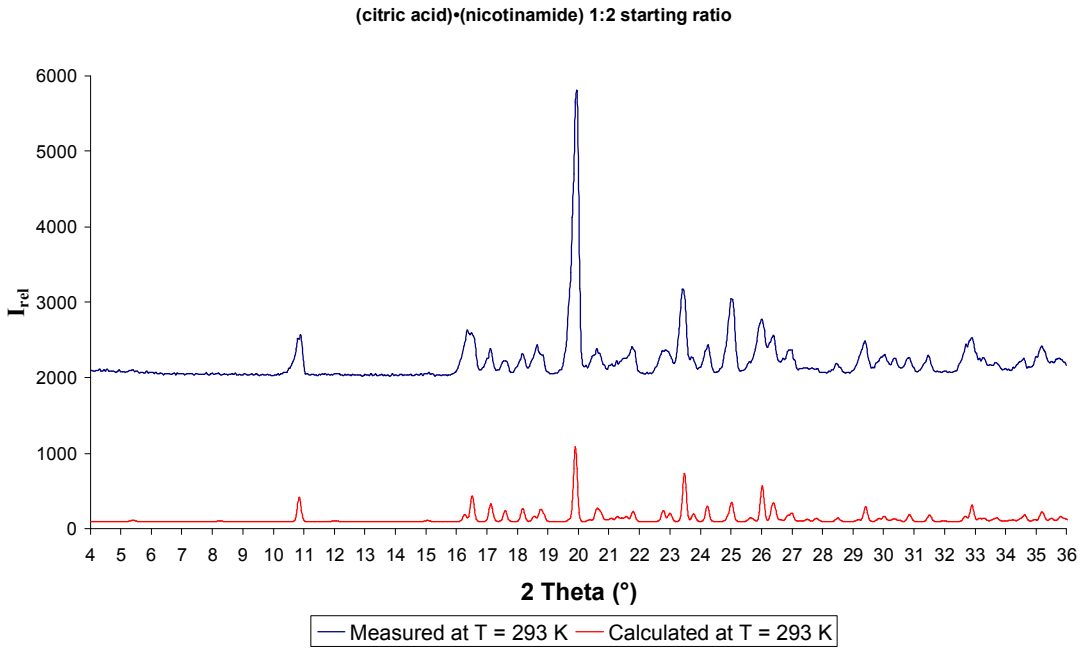

Figure S2: Comparison of powder pattern obtained from co-crystallizing citric acid and nicotinamide in a 1:2 ratio, and that calculated from the single crystal structure.

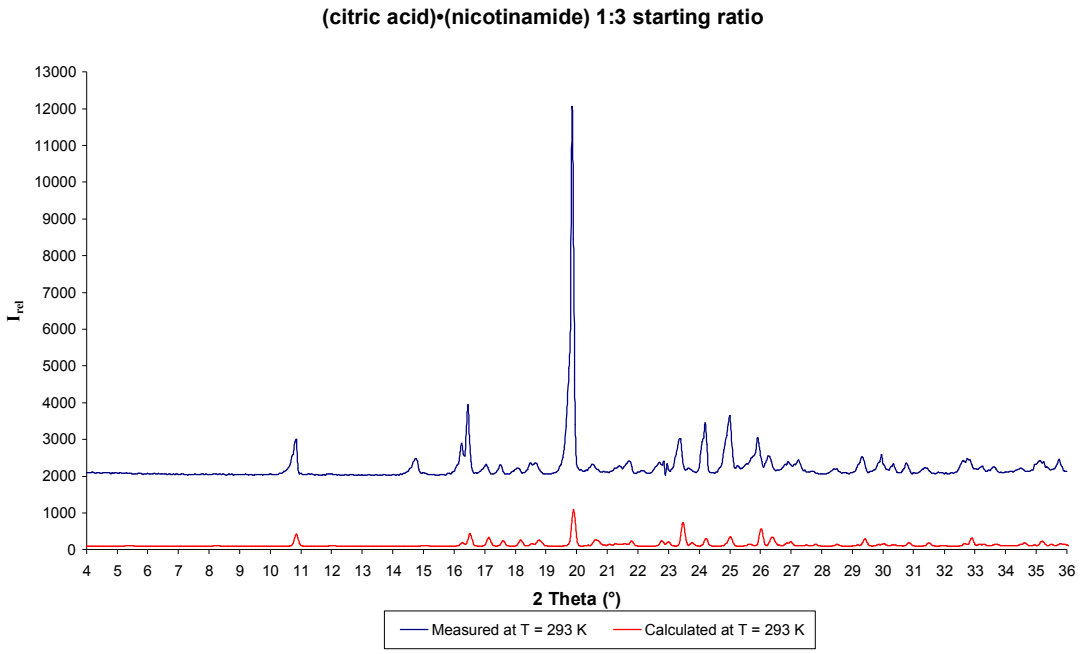

Figure S3: Comparison of powder pattern obtained from co-crystallizing citric acid and nicotinamide in a 1:3 ratio, and that calculated from the single crystal structure.

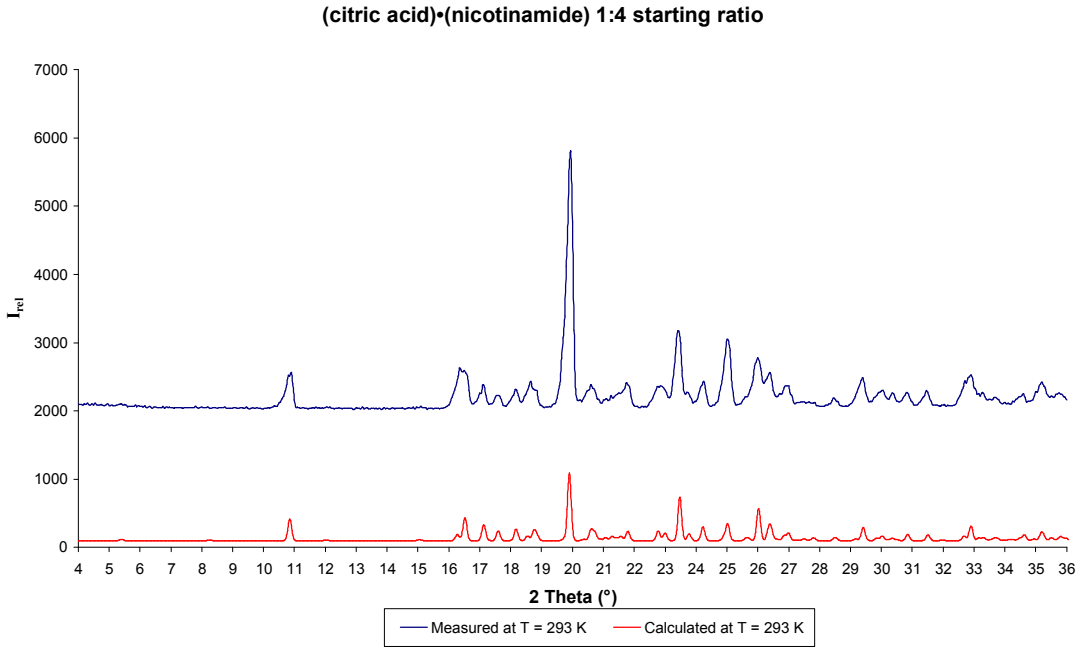

Figure S4: Comparison of powder pattern obtained from co-crystallizing citric acid and nicotinamide in a 1:4 ratio, and that calculated from the single crystal structure.

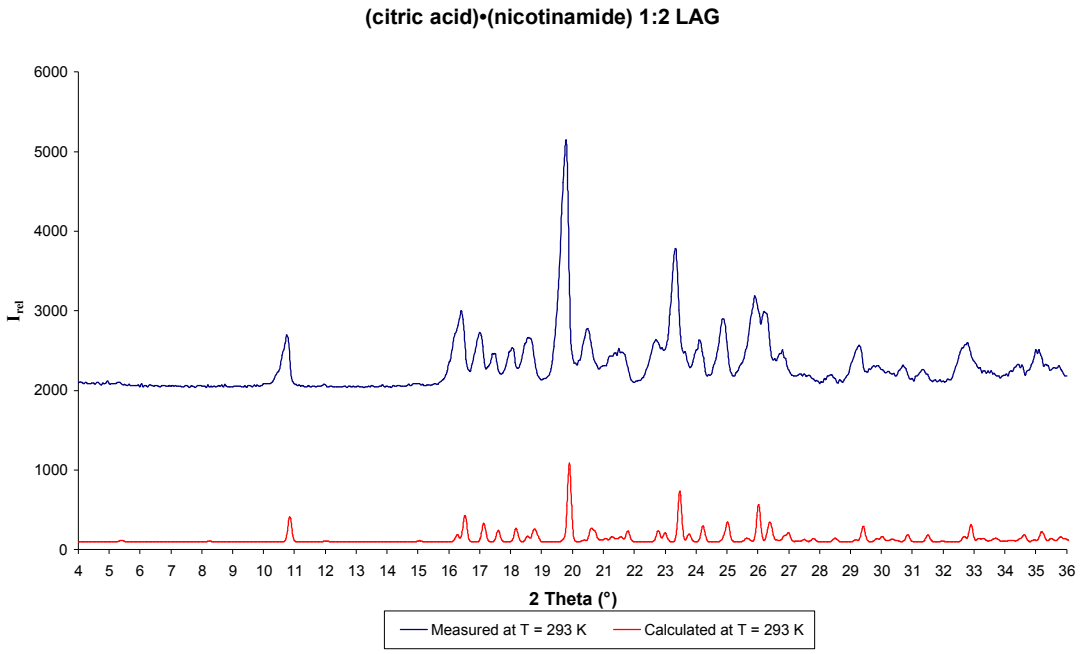

Figure S5: Comparison of powder pattern obtained from liquid-assisted grinding of citric acid and nicotinamide in a 1:2 ratio, and that calculated from the single crystal structure.

Table S1. Crystal data and structure refinement for **1**.

Identification code	8anp102s	
Empirical formula	C18 H20 N4 O9	
Formula weight	436.38	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 5.3769(4) Å	α= 101.325(3)°.
	b = 11.3121(8) Å	β= 96.441(3)°.
	c = 16.9006(11) Å	γ = 103.112(3)°.
Volume	968.36(12) $Å^3$	
Z	2	
Density (calculated)	1.497 Mg/m^3	
Absorption coefficient	0.122 mm^{-1}	
F(000)	456	
Crystal size	0.45 x 0.16 x 0.14 mm^3	
Theta range for data collection	1.90 to 28.00°.	
Index ranges	-7<=h<=6, -14<=k<=14, -22<=l<=22	
Reflections collected	11850	
Independent reflections	4634 [R(int) = 0.0282]	
Completeness to theta = 28.00°	99.6 %	
Absorption correction	Integration	
Max. and min. transmission	0.99 and 0.94	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4634 / 0 / 304	
Goodness-of-fit on F^2	1.006	
Final R indices [I>2sigma(I)]	R1 = 0.0424, wR2 = 0.1043	
R indices (all data)	R1 = 0.0788, wR2 = 0.1224	
Largest diff. peak and hole	0.238 and -0.258 $e.Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	-813(3)	2680(2)	9284(1)	31(1)
C(2)	1313(3)	3681(2)	9376(1)	34(1)
C(3)	-1008(4)	4714(2)	8672(1)	38(1)
C(4)	-3218(4)	3773(2)	8552(1)	40(1)
C(5)	-3147(3)	2743(2)	8873(1)	36(1)
C(6)	-493(3)	1559(2)	9589(1)	34(1)
N(1)	-2301(4)	1069(2)	9986(1)	50(1)
N(2)	1237(3)	4688(1)	9089(1)	36(1)
O(1)	1353(2)	1124(1)	9454(1)	45(1)
C(7)	-873(3)	7523(2)	4048(1)	33(1)
C(8)	195(3)	7604(2)	4848(1)	36(1)
C(9)	2266(4)	6087(2)	4457(1)	47(1)
C(10)	1293(5)	5941(2)	3644(1)	59(1)
C(11)	-287(4)	6672(2)	3439(1)	50(1)
C(12)	-2594(3)	8314(2)	3828(1)	34(1)
N(3)	-3349(4)	9024(2)	4423(1)	48(1)
N(4)	1742(3)	6905(1)	5048(1)	39(1)
O(2)	-3262(3)	8296(1)	3100(1)	46(1)
C(13)	4993(3)	6762(2)	8300(1)	30(1)
C(14)	6406(3)	8016(2)	8190(1)	30(1)
C(15)	7862(3)	7907(1)	7472(1)	28(1)
C(16)	9276(3)	9204(2)	7350(1)	33(1)
C(17)	7549(3)	9874(2)	6960(1)	33(1)
C(18)	6127(3)	7200(2)	6657(1)	30(1)
O(3)	4523(3)	6796(1)	9058(1)	40(1)
O(4)	4344(3)	5829(1)	7762(1)	43(1)
O(5)	6414(3)	10500(1)	7475(1)	46(1)
O(6)	7223(3)	9826(1)	6226(1)	43(1)
O(7)	3858(2)	7442(1)	6561(1)	36(1)
O(8)	6939(3)	6570(1)	6133(1)	47(1)
O(10)	9768(2)	7281(1)	7668(1)	38(1)

Table S3. Bond lengths [Å] and angles [°] for **1**.

C(1)-C(2)	1.385(2)
C(1)-C(5)	1.388(2)
C(1)-C(6)	1.496(2)
C(2)-N(2)	1.330(2)
C(2)-H(2)	0.9300
C(3)-N(2)	1.337(2)
C(3)-C(4)	1.369(3)
C(3)-H(3C)	0.9300
C(4)-C(5)	1.385(3)
C(4)-H(4)	0.9300
C(5)-H(5A)	0.9300
C(6)-O(1)	1.227(2)
C(6)-N(1)	1.323(2)
N(1)-H(1S)	0.87(2)
N(1)-H(1A)	0.94(2)
C(7)-C(11)	1.380(2)
C(7)-C(8)	1.385(2)
C(7)-C(12)	1.491(2)
C(8)-N(4)	1.332(2)
C(8)-H(8)	0.9300
C(9)-N(4)	1.324(2)
C(9)-C(10)	1.377(3)
C(9)-H(9A)	0.9300
C(10)-C(11)	1.375(3)
C(10)-H(10A)	0.9300
C(11)-H(11)	0.9300
C(12)-O(2)	1.237(2)
C(12)-N(3)	1.322(2)
N(3)-H(3S)	0.89(3)
N(3)-H(3A)	0.89(2)
N(4)-H(7)	1.49(2)
C(13)-O(4)	1.204(2)
C(13)-O(3)	1.328(2)
C(13)-C(14)	1.506(2)
C(14)-C(15)	1.516(2)
C(14)-H(14A)	0.9700

C(14)-H(14B)	0.9700
C(15)-O(10)	1.4167(18)
C(15)-C(18)	1.532(2)
C(15)-C(16)	1.556(2)
C(16)-C(17)	1.500(2)
C(16)-H(16A)	0.9700
C(16)-H(16B)	0.9700
C(17)-O(6)	1.223(2)
C(17)-O(5)	1.306(2)
C(18)-O(8)	1.2107(19)
C(18)-O(7)	1.309(2)
O(3)-H(3)	1.03(2)
O(5)-H(5)	0.91(3)
O(7)-H(7)	1.09(2)
O(10)-H(10)	0.84(2)

C(2)-C(1)-C(5)	117.74(15)
C(2)-C(1)-C(6)	119.46(15)
C(5)-C(1)-C(6)	122.73(15)
N(2)-C(2)-C(1)	123.56(16)
N(2)-C(2)-H(2)	118.2
C(1)-C(2)-H(2)	118.2
N(2)-C(3)-C(4)	122.96(16)
N(2)-C(3)-H(3C)	118.5
C(4)-C(3)-H(3C)	118.5
C(3)-C(4)-C(5)	119.00(17)
C(3)-C(4)-H(4)	120.5
C(5)-C(4)-H(4)	120.5
C(4)-C(5)-C(1)	118.88(17)
C(4)-C(5)-H(5A)	120.6
C(1)-C(5)-H(5A)	120.6
O(1)-C(6)-N(1)	123.10(17)
O(1)-C(6)-C(1)	120.18(15)
N(1)-C(6)-C(1)	116.71(16)
C(6)-N(1)-H(1S)	118.8(15)
C(6)-N(1)-H(1A)	119.8(14)
H(1S)-N(1)-H(1A)	121(2)
C(2)-N(2)-C(3)	117.79(15)

C(11)-C(7)-C(8)	117.65(16)
C(11)-C(7)-C(12)	119.64(15)
C(8)-C(7)-C(12)	122.71(15)
N(4)-C(8)-C(7)	123.00(16)
N(4)-C(8)-H(8)	118.5
C(7)-C(8)-H(8)	118.5
N(4)-C(9)-C(10)	122.58(18)
N(4)-C(9)-H(9A)	118.7
C(10)-C(9)-H(9A)	118.7
C(11)-C(10)-C(9)	118.75(19)
C(11)-C(10)-H(10A)	120.6
C(9)-C(10)-H(10A)	120.6
C(10)-C(11)-C(7)	119.52(17)
C(10)-C(11)-H(11)	120.2
C(7)-C(11)-H(11)	120.2
O(2)-C(12)-N(3)	121.82(16)
O(2)-C(12)-C(7)	119.68(15)
N(3)-C(12)-C(7)	118.50(15)
C(12)-N(3)-H(3S)	119.3(14)
C(12)-N(3)-H(3A)	124.5(15)
H(3S)-N(3)-H(3A)	115(2)
C(9)-N(4)-C(8)	118.50(15)
C(9)-N(4)-H(7)	122.3(8)
C(8)-N(4)-H(7)	119.0(8)
O(4)-C(13)-O(3)	123.29(15)
O(4)-C(13)-C(14)	124.05(15)
O(3)-C(13)-C(14)	112.65(14)
C(13)-C(14)-C(15)	112.32(13)
C(13)-C(14)-H(14A)	109.1
C(15)-C(14)-H(14A)	109.1
C(13)-C(14)-H(14B)	109.1
C(15)-C(14)-H(14B)	109.1
H(14A)-C(14)-H(14B)	107.9
O(10)-C(15)-C(14)	106.03(12)
O(10)-C(15)-C(18)	110.35(13)
C(14)-C(15)-C(18)	113.49(13)
O(10)-C(15)-C(16)	107.83(13)
C(14)-C(15)-C(16)	112.22(13)

C(18)-C(15)-C(16)	106.82(13)
C(17)-C(16)-C(15)	114.70(14)
C(17)-C(16)-H(16A)	108.6
C(15)-C(16)-H(16A)	108.6
C(17)-C(16)-H(16B)	108.6
C(15)-C(16)-H(16B)	108.6
H(16A)-C(16)-H(16B)	107.6
O(6)-C(17)-O(5)	123.32(16)
O(6)-C(17)-C(16)	122.85(16)
O(5)-C(17)-C(16)	113.83(14)
O(8)-C(18)-O(7)	124.46(16)
O(8)-C(18)-C(15)	121.00(15)
O(7)-C(18)-C(15)	114.21(14)
C(13)-O(3)-H(3)	108.6(12)
C(17)-O(5)-H(5)	113.6(15)
C(18)-O(7)-H(7)	109.4(11)
C(15)-O(10)-H(10)	110.8(16)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	37(1)	30(1)	31(1)	9(1)	10(1)	13(1)
C(2)	33(1)	38(1)	35(1)	14(1)	8(1)	12(1)
C(3)	47(1)	37(1)	38(1)	18(1)	12(1)	20(1)
C(4)	38(1)	46(1)	40(1)	12(1)	4(1)	19(1)
C(5)	35(1)	33(1)	40(1)	7(1)	7(1)	10(1)
C(6)	37(1)	27(1)	38(1)	9(1)	7(1)	8(1)
N(1)	54(1)	43(1)	75(1)	36(1)	31(1)	24(1)
N(2)	41(1)	33(1)	39(1)	16(1)	11(1)	11(1)
O(1)	43(1)	39(1)	67(1)	25(1)	18(1)	19(1)
C(7)	38(1)	30(1)	32(1)	9(1)	2(1)	10(1)
C(8)	41(1)	38(1)	31(1)	9(1)	3(1)	15(1)
C(9)	59(1)	40(1)	46(1)	9(1)	-2(1)	26(1)
C(10)	87(2)	52(1)	40(1)	-3(1)	-5(1)	42(1)
C(11)	70(1)	48(1)	33(1)	1(1)	-9(1)	30(1)
C(12)	37(1)	35(1)	32(1)	10(1)	2(1)	11(1)
N(3)	61(1)	64(1)	34(1)	14(1)	8(1)	39(1)
N(4)	43(1)	41(1)	33(1)	11(1)	-1(1)	15(1)
O(2)	61(1)	54(1)	30(1)	12(1)	0(1)	32(1)
C(13)	29(1)	33(1)	32(1)	11(1)	1(1)	12(1)
C(14)	33(1)	30(1)	27(1)	8(1)	2(1)	9(1)
C(15)	27(1)	29(1)	31(1)	12(1)	2(1)	12(1)
C(16)	32(1)	36(1)	33(1)	12(1)	4(1)	8(1)
C(17)	38(1)	28(1)	32(1)	10(1)	5(1)	6(1)
C(18)	35(1)	29(1)	31(1)	11(1)	5(1)	13(1)
O(3)	48(1)	39(1)	32(1)	13(1)	8(1)	5(1)
O(4)	56(1)	33(1)	37(1)	7(1)	5(1)	6(1)
O(5)	66(1)	49(1)	34(1)	10(1)	6(1)	34(1)
O(6)	57(1)	48(1)	31(1)	16(1)	9(1)	24(1)
O(7)	35(1)	47(1)	30(1)	8(1)	0(1)	19(1)
O(8)	53(1)	48(1)	41(1)	0(1)	6(1)	25(1)
O(10)	34(1)	46(1)	42(1)	19(1)	5(1)	22(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **1**.

	x	y	z	U(eq)
H(2)	2880	3648	9655	40
H(3C)	-1071	5403	8455	45
H(4)	-4745	3825	8258	48
H(5A)	-4637	2105	8814	43
H(1S)	-2130(40)	440(20)	10188(14)	60
H(1A)	-3580(50)	1480(20)	10115(14)	60
H(8)	-185	8174	5264	43
H(9A)	3333	5592	4595	56
H(10A)	1697	5359	3242	70
H(11)	-956	6594	2894	60
H(3S)	-4530(50)	9430(20)	4299(13)	58
H(3A)	-2960(40)	9040(20)	4955(15)	58
H(14A)	7620	8457	8686	36
H(14B)	5169	8503	8106	36
H(16A)	10150	9726	7879	40
H(16B)	10592	9094	7014	40
H(3)	3380(40)	5940(20)	9074(13)	60
H(5)	5340(50)	10890(20)	7234(15)	70
H(7)	3000(40)	7147(19)	5918(13)	54
H(10)	10410(40)	7040(20)	7256(14)	56

Table S6. Torsion angles [°] for **1**.

C(5)-C(1)-C(2)-N(2)	-0.5(2)
C(6)-C(1)-C(2)-N(2)	176.53(15)
N(2)-C(3)-C(4)-C(5)	0.0(3)
C(3)-C(4)-C(5)-C(1)	-2.1(3)
C(2)-C(1)-C(5)-C(4)	2.3(2)
C(6)-C(1)-C(5)-C(4)	-174.59(16)
C(2)-C(1)-C(6)-O(1)	-44.5(2)
C(5)-C(1)-C(6)-O(1)	132.35(19)
C(2)-C(1)-C(6)-N(1)	136.70(18)
C(5)-C(1)-C(6)-N(1)	-46.4(2)
C(1)-C(2)-N(2)-C(3)	-1.6(2)
C(4)-C(3)-N(2)-C(2)	1.8(2)
C(11)-C(7)-C(8)-N(4)	0.0(3)
C(12)-C(7)-C(8)-N(4)	-179.69(16)
N(4)-C(9)-C(10)-C(11)	-0.1(4)
C(9)-C(10)-C(11)-C(7)	-0.5(3)
C(8)-C(7)-C(11)-C(10)	0.5(3)
C(12)-C(7)-C(11)-C(10)	-179.8(2)
C(11)-C(7)-C(12)-O(2)	-7.5(3)
C(8)-C(7)-C(12)-O(2)	172.18(17)
C(11)-C(7)-C(12)-N(3)	172.94(18)
C(8)-C(7)-C(12)-N(3)	-7.4(3)
C(10)-C(9)-N(4)-C(8)	0.6(3)
C(7)-C(8)-N(4)-C(9)	-0.5(3)
O(4)-C(13)-C(14)-C(15)	-23.2(2)
O(3)-C(13)-C(14)-C(15)	157.05(14)
C(13)-C(14)-C(15)-O(10)	-63.62(17)
C(13)-C(14)-C(15)-C(18)	57.67(18)
C(13)-C(14)-C(15)-C(16)	178.90(13)
O(10)-C(15)-C(16)-C(17)	167.00(13)
C(14)-C(15)-C(16)-C(17)	-76.59(17)
C(18)-C(15)-C(16)-C(17)	48.40(18)
C(15)-C(16)-C(17)-O(6)	-95.4(2)
C(15)-C(16)-C(17)-O(5)	83.98(18)
O(10)-C(15)-C(18)-O(8)	-28.4(2)
C(14)-C(15)-C(18)-O(8)	-147.26(15)

C(16)-C(15)-C(18)-O(8)	88.53(18)
O(10)-C(15)-C(18)-O(7)	157.93(13)
C(14)-C(15)-C(18)-O(7)	39.09(18)
C(16)-C(15)-C(18)-O(7)	-85.12(16)

Symmetry transformations used to generate equivalent atoms:

Table S7. Hydrogen bonds for **1** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1S)...O(1)#1	0.87(2)	2.09(3)	2.949(2)	171(2)
N(1)-H(1A)...O(3)#2	0.94(2)	2.36(2)	3.176(2)	146(2)
N(3)-H(3S)...O(6)#3	0.89(3)	2.04(3)	2.917(2)	168(2)
N(3)-H(3A)...O(6)#4	0.89(2)	2.14(2)	2.962(2)	153(2)
O(3)-H(3)...N(2)	1.03(2)	1.62(2)	2.640(2)	172(2)
O(5)-H(5)...O(2)#3	0.91(3)	1.71(3)	2.620(2)	173(2)
O(7)-H(7)...N(4)	1.09(2)	1.49(2)	2.574(2)	172(2)
O(10)-H(10)...O(7)#5	0.84(2)	2.31(2)	3.040(2)	146(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z+2 #2 -x,-y+1,-z+2 #3 -x,-y+2,-z+1

#4 x-1,y,z #5 x+1,y,z