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2-Amino-6-chloropyridine–glutaric acid (1/1)

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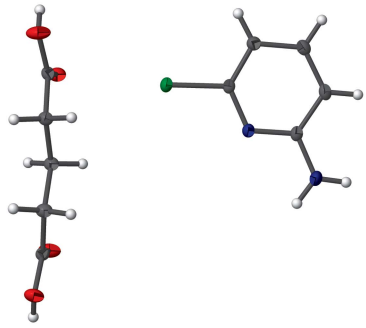
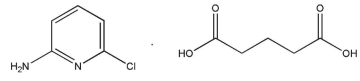
Structural data: full structural data are available from iucrdata.iucr.org

In the title 1:1 co-crystal [systematic name: 6-chloropyridin-2-amine–pentanedioic acid (1/1)], $C_5H_5ClN_2{\cdot}C_5H_8O_4$, the pyridine ring is essentially planar, with a maximum deviation of 0.003 (1) Å. The base and acid molecules are linked *via* N—H···O and O—H···N hydrogen bonds, while inversion-related acid molecules are linked *via* pairs of O—H···O hydrogen bonds. These interactions together with a C—H···O hydrogen bond connect the two components, forming (001) sheets.

3D view



Chemical scheme



Structure description

In order to study hydrogen-bonding interactions in pyridine–carboxy acid systems, the crystal structure determination of the title compound was carried out. Some related crystal structures have previously been reported, *viz*. 2-amino-5-methylpyridinium 4-carboxybutanoate (Hemamalini & Fun, 2010), 2,6-diamino-4-chloropyrimidinium 4-carboxybutanoate (Edison *et al.*, 2014), pyrimidin-2-amine–glutaric acid (1/1) and bis(2-aminopyrimidinium)glutarate–glutaric acid (1/2) (Odiase *et al.*, 2015).

As expected, the pyridine ring of the title compound is essentially planar, with a maximum deviation of 0.004 (1) Å for atom C1. The backbone conformation of the acid molecule can be described by the torsion angles C6—C7—C8—C9 [−174.76 (9)°] and C7—C8—C9—C10 [171.92 (9)°], which indicates a fully extended conformation of the molecule. The dihedral angle between the CO_2H groups is 13.8 (10)°.. As evident from the torsion angles, the backbone exhibits a fully extended conformation of the two carboxyl groups (Fig. 1). In the crystal, the N1 atom and the 2-amino group (N2) are linked to the carboxyl oxygen atoms (O3 and O4) *via* O—H···N and N—H···O

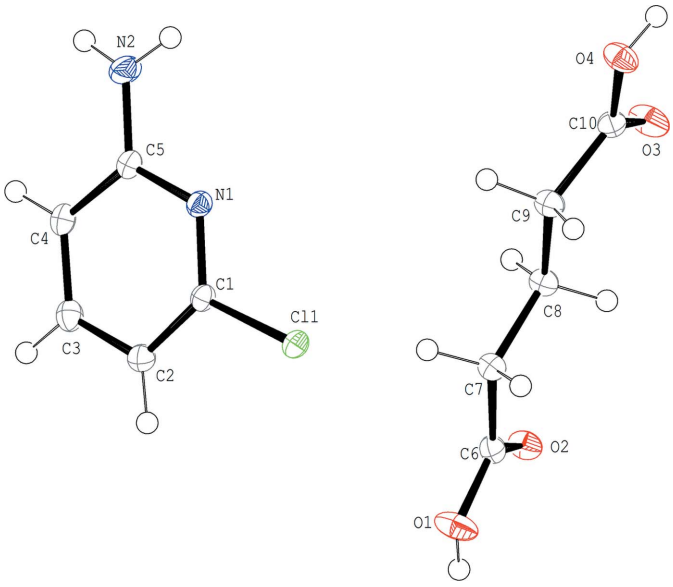


Figure 1
The asymmetric unit of the title compound. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

hydrogen bonds with an $R_2^2(8)$ ring motif. The acid and base molecules are further linked by O—H···O and C—H···O hydrogen bonds (Table 1), forming (001) sheets (Fig. 2)

Synthesis and crystallization

Hot methanol solutions (20 ml) of 2-amino-6-chloropyridine (34 mg, Aldrich) and glutaric acid (34 mg, Merck) were mixed. The resulting solution was allowed to cool slowly at room temperature and crystals of the title compound appeared after a few days.

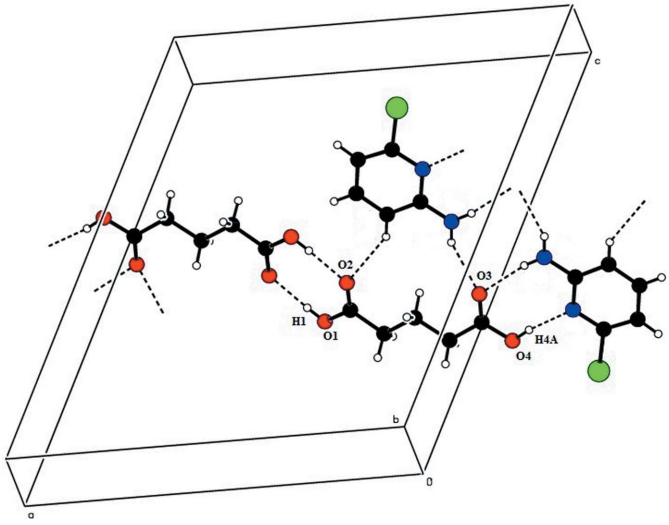


Figure 2
A packing view of the title compound, showing the sheet structure formed by O—H···O, O—H···N, N—H···O and C—H···O hydrogen bonds (dashed lines).

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···O2^{i}	0.93	2.55	3.3711 (13)	147
N2—H2A···O3^{ii}	0.87 (1)	2.08 (1)	2.9443 (13)	171 (2)
N2—H2B···O3^{i}	0.87 (1)	2.18 (1)	2.9525 (13)	147 (1)
O1—H1A···O2^{iii}	0.83 (1)	1.82 (1)	2.6433 (12)	173 (2)
O4—H4A···N1^{iv}	0.83 (1)	1.93 (1)	2.7545 (12)	171 (2)

Symmetry codes: (i) $x, -y+\frac{3}{2}, z-\frac{1}{2}$; (ii) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$; (iii) $-x+1, -y, -z+1$; (iv) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_5H_5ClN_2·C_5H_8O_4$
M_r	260.67
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	14.7115 (16), 4.9598 (6), 17.3105 (19)
β (°)	112.960 (2)
V (Å^3)	1163.0 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.33
Crystal size (mm)	0.80 × 0.30 × 0.04
Data collection	
Diffractometer	Bruker *SMART* APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2012)
T_{min}, T_{max}	0.774, 0.987
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14500, 3966, 3264
R_{int}	0.036
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.742
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.033, 0.094, 0.93
No. of reflections	3966
No. of parameters	170
No. of restraints	4
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.49, −0.29

Computer programs: *APEX2* and *SAINT* (Bruker, 2012), *SHELXS2016* (Sheldrick, 2015*a*), *SHELXL2016* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

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full crystallographic data

IUCrData (2019). **4**, x190781 [https://doi.org/10.1107/S2414314619007818]

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6-Chloropyridin-2-amine–pentanedioic acid (1/1)

Crystal data

$C_5H_5ClN_2·C_5H_8O_4$
M_r = 260.67
Monoclinic, $P2_1/c$
a = 14.7115 (16) Å
b = 4.9598 (6) Å
c = 17.3105 (19) Å
β = 112.960 (2)°
V = 1163.0 (2) Å^3
Z = 4
$F(000)$ = 544
D_x = 1.489 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3966 reflections
θ = 3.1–31.8°
μ = 0.33 mm^{-1}
T = 296 K
Plate, yellow
0.80 × 0.30 × 0.04 mm

Data collection

Bruker SMART APEXII CCD diffractometer
ω and φ scan
Absorption correction: multi-scan (*SADABS*; Bruker, 2012)
T_{min} = 0.774, T_{max} = 0.987
14500 measured reflections
3966 independent reflections
3264 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 31.8°, θ_{min} = 3.1°
h = −21→21
k = −7→6
l = −25→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.094
S = 0.93
3966 reflections
170 parameters
4 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0538P)^2 + 0.4259P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. The C-bound H atoms were positioned geometrically (C—H = 0.93 or 0.97 Å) and were refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C). Other H atoms were located in a difference map and refined with bond length restraints [O—H = 0.83 (1) Å and N—H = 0.88 (1) Å].

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.32219 (7)	0.5358 (2)	0.18568 (6)	0.01383 (18)
C2	0.40778 (8)	0.6161 (2)	0.17751 (7)	0.0171 (2)
H2	0.468418	0.536117	0.208091	0.021*
C3	0.39787 (8)	0.8254 (2)	0.12033 (7)	0.0183 (2)
H3	0.453167	0.888572	0.112474	0.022*
C4	0.30710 (8)	0.9376 (2)	0.07589 (6)	0.0171 (2)
H4	0.300439	1.076883	0.038085	0.021*
C5	0.22388 (8)	0.8382 (2)	0.08852 (6)	0.01566 (19)
C6	0.36785 (8)	−0.0963 (2)	0.42745 (7)	0.0158 (2)
C7	0.26506 (7)	−0.1901 (2)	0.37424 (7)	0.01589 (19)
H7A	0.257736	−0.376398	0.387846	0.019*
H7B	0.255794	−0.182763	0.315646	0.019*
C8	0.18569 (7)	−0.0211 (2)	0.38679 (7)	0.01630 (19)
H8A	0.198131	−0.014805	0.446066	0.020*
H8B	0.188724	0.161843	0.368117	0.020*
C9	0.08316 (8)	−0.1353 (2)	0.33855 (7)	0.0173 (2)
H9A	0.067398	−0.118190	0.278884	0.021*
H9B	0.083179	−0.325822	0.351259	0.021*
C10	0.00447 (7)	0.0044 (2)	0.35926 (6)	0.0161 (2)
N1	0.23222 (6)	0.6371 (2)	0.14376 (5)	0.01474 (17)
N2	0.13245 (7)	0.9357 (2)	0.04534 (7)	0.0232 (2)
H2A	0.0834 (10)	0.882 (4)	0.0580 (11)	0.039 (5)*
H2B	0.1237 (11)	1.074 (2)	0.0120 (9)	0.026 (4)*
O1	0.43745 (6)	−0.2565 (2)	0.42360 (6)	0.0258 (2)
H1A	0.4925 (9)	−0.197 (4)	0.4543 (10)	0.039 (5)*
O2	0.38508 (6)	0.10702 (17)	0.47067 (5)	0.01919 (17)
O3	0.02085 (6)	0.19918 (19)	0.40576 (6)	0.0255 (2)
O4	−0.08387 (6)	−0.10152 (19)	0.32075 (5)	0.02091 (18)
H4A	−0.1240 (12)	−0.019 (4)	0.3347 (12)	0.052 (6)*
Cl1	0.32782 (2)	0.28122 (6)	0.25664 (2)	0.01679 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0167 (4)	0.0121 (5)	0.0126 (4)	−0.0002 (4)	0.0056 (3)	0.0002 (3)
C2	0.0156 (4)	0.0188 (5)	0.0165 (4)	−0.0003 (4)	0.0057 (4)	0.0007 (4)
C3	0.0196 (5)	0.0193 (6)	0.0169 (4)	−0.0036 (4)	0.0082 (4)	−0.0008 (4)
C4	0.0215 (5)	0.0160 (5)	0.0148 (4)	−0.0023 (4)	0.0081 (4)	0.0007 (4)
C5	0.0184 (4)	0.0149 (5)	0.0135 (4)	−0.0001 (4)	0.0061 (4)	0.0012 (4)
C6	0.0168 (4)	0.0154 (5)	0.0167 (4)	−0.0001 (4)	0.0081 (4)	0.0004 (4)
C7	0.0153 (4)	0.0155 (5)	0.0170 (4)	−0.0010 (4)	0.0064 (4)	−0.0019 (4)
C8	0.0158 (4)	0.0149 (5)	0.0181 (4)	−0.0003 (4)	0.0065 (4)	−0.0021 (4)
C9	0.0155 (4)	0.0174 (5)	0.0186 (5)	−0.0002 (4)	0.0061 (4)	−0.0038 (4)
C10	0.0150 (4)	0.0164 (5)	0.0155 (4)	−0.0005 (4)	0.0042 (3)	−0.0005 (4)
N1	0.0153 (4)	0.0147 (4)	0.0139 (4)	0.0001 (3)	0.0054 (3)	0.0017 (3)

N2	0.0187 (4)	0.0256 (6)	0.0246 (5)	0.0033 (4)	0.0075 (4)	0.0126 (4)
O1	0.0141 (4)	0.0260 (5)	0.0345 (5)	0.0004 (3)	0.0063 (3)	−0.0149 (4)
O2	0.0169 (3)	0.0168 (4)	0.0231 (4)	−0.0004 (3)	0.0070 (3)	−0.0051 (3)
O3	0.0173 (4)	0.0266 (5)	0.0316 (5)	−0.0025 (3)	0.0083 (3)	−0.0143 (4)
O4	0.0148 (3)	0.0227 (5)	0.0254 (4)	−0.0033 (3)	0.0081 (3)	−0.0081 (3)
Cl1	0.01809 (12)	0.01660 (13)	0.01572 (12)	0.00172 (9)	0.00664 (9)	0.00420 (9)

Geometric parameters (Å, º)

C1—N1	1.3346 (13)	C7—H7A	0.9700
C1—C2	1.3794 (14)	C7—H7B	0.9700
C1—Cl1	1.7409 (11)	C8—C9	1.5202 (15)
C2—C3	1.4022 (16)	C8—H8A	0.9700
C2—H2	0.9300	C8—H8B	0.9700
C3—C4	1.3724 (16)	C9—C10	1.5076 (15)
C3—H3	0.9300	C9—H9A	0.9700
C4—C5	1.4137 (14)	C9—H9B	0.9700
C4—H4	0.9300	C10—O3	1.2199 (14)
C5—N2	1.3481 (14)	C10—O4	1.3165 (13)
C5—N1	1.3540 (14)	N2—H2A	0.873 (9)
C6—O2	1.2217 (14)	N2—H2B	0.873 (9)
C6—O1	1.3181 (13)	O1—H1A	0.830 (9)
C6—C7	1.5049 (15)	O4—H4A	0.828 (9)
C7—C8	1.5202 (15)		
N1—C1—C2	125.94 (10)	H7A—C7—H7B	107.8
N1—C1—Cl1	114.88 (7)	C9—C8—C7	111.65 (9)
C2—C1—Cl1	119.18 (8)	C9—C8—H8A	109.3
C1—C2—C3	116.00 (10)	C7—C8—H8A	109.3
C1—C2—H2	122.0	C9—C8—H8B	109.3
C3—C2—H2	122.0	C7—C8—H8B	109.3
C4—C3—C2	120.43 (10)	H8A—C8—H8B	108.0
C4—C3—H3	119.8	C10—C9—C8	112.80 (9)
C2—C3—H3	119.8	C10—C9—H9A	109.0
C3—C4—C5	118.93 (10)	C8—C9—H9A	109.0
C3—C4—H4	120.5	C10—C9—H9B	109.0
C5—C4—H4	120.5	C8—C9—H9B	109.0
N2—C5—N1	116.87 (9)	H9A—C9—H9B	107.8
N2—C5—C4	121.74 (10)	O3—C10—O4	123.51 (10)
N1—C5—C4	121.39 (10)	O3—C10—C9	123.27 (10)
O2—C6—O1	123.27 (10)	O4—C10—C9	113.20 (9)
O2—C6—C7	123.29 (10)	C1—N1—C5	117.31 (9)
O1—C6—C7	113.43 (9)	C5—N2—H2A	119.6 (13)
C6—C7—C8	112.74 (9)	C5—N2—H2B	120.4 (10)
C6—C7—H7A	109.0	H2A—N2—H2B	119.0 (16)
C8—C7—H7A	109.0	C6—O1—H1A	109.8 (13)
C6—C7—H7B	109.0	C10—O4—H4A	109.2 (14)
C8—C7—H7B	109.0		

N1—C1—C2—C3	0.78 (17)	C6—C7—C8—C9	−174.76 (9)
Cl1—C1—C2—C3	−178.87 (8)	C7—C8—C9—C10	171.92 (9)
C1—C2—C3—C4	−0.39 (16)	C8—C9—C10—O3	4.34 (16)
C2—C3—C4—C5	−0.21 (16)	C8—C9—C10—O4	−176.99 (9)
C3—C4—C5—N2	−178.41 (11)	C2—C1—N1—C5	−0.50 (16)
C3—C4—C5—N1	0.52 (16)	Cl1—C1—N1—C5	179.16 (8)
O2—C6—C7—C8	−5.66 (15)	N2—C5—N1—C1	178.80 (10)
O1—C6—C7—C8	173.62 (10)	C4—C5—N1—C1	−0.18 (15)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···O2^{i}	0.93	2.55	3.3711 (13)	147
N2—H2*A*···O3^{ii}	0.87 (1)	2.08 (1)	2.9443 (13)	171 (2)
N2—H2*B*···O3^{i}	0.87 (1)	2.18 (1)	2.9525 (13)	147 (1)
O1—H1*A*···O2^{iii}	0.83 (1)	1.82 (1)	2.6433 (12)	173 (2)
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