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3-Carboxy-2-(piperidin-1-ium-1-yl)propanoate

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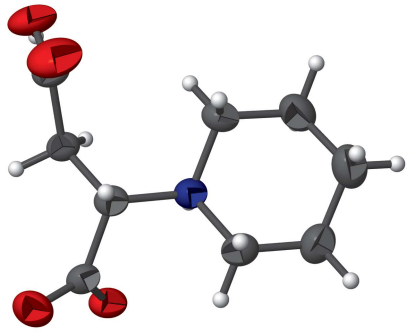
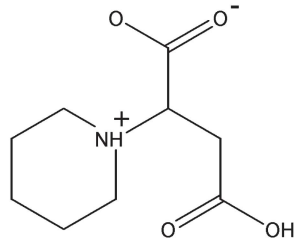
Structural data: full structural data are available from iucrdata.iucr.org

In the zwitterionic title compound, $C_9H_{15}NO_4$, the piperidinium N atom is protonated and the OH group of one of the carboxylate groups is deprotonated. The piperidinium ring adopts a chair conformation. In the crystal, N—H···O and O—H···O hydrogen bonds generate an $R_3^3(15)$ ring motif and link the molecules into infinite chains propagating along [010]. The structure is further consolidated by weak C—H···O interactions to form a three-dimensional network.

3D view



Chemical scheme



Structure description

Piperidine and its derivatives find extensive applications in some areas of biochemistry and material chemistry. They also exhibit good bioactivity (Cardellicchio *et al.* 2010; Huang *et al.* 2008). We report here the synthesis and the crystal structure of the title compound (Fig. 1). The N atom of the the piperidinium ring is protonated while the OH substituent of one of the carboxylate groups is deprotonated. The geometric parameters are comparable to those reported for similar structures (Aravindhan *et al.*, 2009; Sankar *et al.*, 2014).

The piperidine ring (N1/C1–C5) adopts a chair conformation with puckering parameters of Q = 0.579 (3) Å; θ = 1.0 (3)° and φ = 134 (15)°. An intramolecular N—H···O hydrogen bond occurs (Table 1). In the crystal, N—H···O and O—H···O hydrogen bonds generate $R_3^3(15)$ ring motifs (Fig. 2) and link the molecules into infinite chains along [010]. The structure is further consolidated by weak C—H···O interactions (Table 1 and Fig. 3) to form a three-dimensional network.

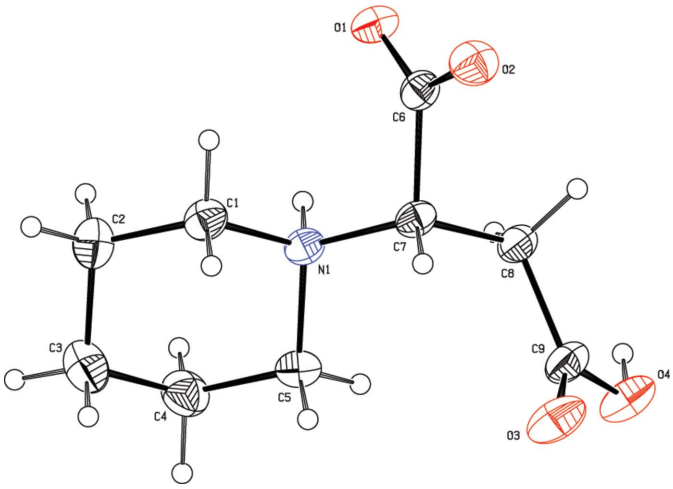


Figure 1
The molecular structure of the title compound, with atom labelling and 30% probability displacement ellipsoids.

Synthesis and crystallization

The title compound was synthesized from piperidine (0.85 g) and maleic acid (1.16 g) in a methanol:water mixed solvent system. Colourless block-like crystals suitable for single-crystal X-ray diffraction were grown by slow evaporation from methanol:water (1:1) mixed solvent.

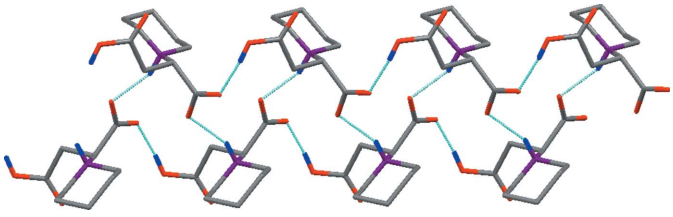


Figure 2
A partial packing diagram showing the ring motif.

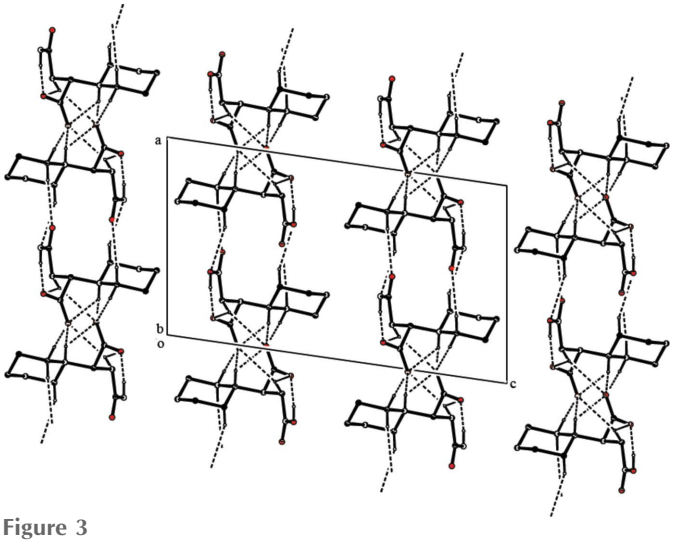


Figure 3
Crystal packing of the title compound viewed along the *b* axis. Hydrogen bonds (see Table 1) are shown as dashed lines and C-bound H atoms have been omitted for clarity.

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1	0.89 (1)	2.42 (2)	2.736 (2)	101 (2)
N1—H1···O1^{i}	0.89 (1)	1.93 (1)	2.759 (2)	154 (2)
O4—H4···O2^{ii}	0.83 (1)	1.73 (1)	2.557 (2)	173 (3)
C1—H1*A*···O1^{iii}	0.97	2.60	3.528 (3)	160
C1—H1*B*···O3^{iv}	0.97	2.44	3.381 (3)	163
C5—H5*A*···O4^{iv}	0.97	2.51	3.439 (3)	161
C8—H8*A*···O2^{ii}	0.97	2.45	3.142 (3)	128
C8—H8*A*···O1^{i}	0.97	2.55	3.368 (2)	143

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_9H_{15}NO_4$
M_r	201.22
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	295
a, b, c (Å)	9.8364 (8), 5.9731 (5), 17.0805 (15)
β (°)	98.152 (5)
V (Å^3)	993.40 (15)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.11
Crystal size (mm)	0.24 × 0.22 × 0.18
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)
T_{min}, T_{max}	0.975, 0.981
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8624, 2431, 1446
R_{int}	0.054
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.668
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.057, 0.172, 1.04
No. of reflections	2431
No. of parameters	134
No. of restraints	2
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.28, −0.19

Computer programs: *APEX2* and *SAINT* (Bruker, 2004), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

Refinement

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

Acknowledgements

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full crystallographic data

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Crystal data

$C_9H_{15}NO_4$
M_r = 201.22
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 9.8364 (8) Å
b = 5.9731 (5) Å
c = 17.0805 (15) Å
β = 98.152 (5)°
V = 993.40 (15) Å^3
Z = 4
$F(000)$ = 432
D_x = 1.345 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5733 reflections
θ = 2.1–28.3°
μ = 0.11 mm^{-1}
T = 295 K
Block, colourless
0.24 × 0.22 × 0.18 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.975, T_{max} = 0.981
8624 measured reflections
2431 independent reflections
1446 reflections with $I > 2\sigma(I)$
R_{int} = 0.054
θ_{max} = 28.4°, θ_{min} = 2.1°
h = −9→13
k = −7→7
l = −22→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.172
S = 1.04
2431 reflections
134 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.090P)^2 + 0.0823P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 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. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.2180 (2)	0.4085 (3)	0.85245 (13)	0.0411 (5)
H1A	0.1439	0.5094	0.8324	0.049*
H1B	0.3042	0.4866	0.8513	0.049*
C2	0.2051 (3)	0.3451 (4)	0.93646 (14)	0.0516 (6)
H2A	0.1164	0.2757	0.9381	0.062*
H2B	0.2103	0.4788	0.9690	0.062*
C3	0.3179 (3)	0.1844 (4)	0.96931 (15)	0.0592 (7)
H3A	0.4066	0.2570	0.9714	0.071*
H3B	0.3060	0.1407	1.0226	0.071*
C4	0.3125 (3)	−0.0200 (4)	0.91702 (15)	0.0539 (6)
H4A	0.2267	−0.0985	0.9187	0.065*
H4B	0.3870	−0.1203	0.9369	0.065*
C5	0.3241 (2)	0.0422 (4)	0.83234 (14)	0.0421 (5)
H5A	0.4133	0.1089	0.8299	0.051*
H5B	0.3167	−0.0918	0.7999	0.051*
C6	0.0979 (2)	0.4225 (3)	0.68531 (12)	0.0369 (5)
C7	0.22115 (18)	0.2712 (3)	0.71628 (12)	0.0344 (5)
H7	0.3069	0.3526	0.7138	0.041*
C8	0.21416 (19)	0.0678 (3)	0.66188 (13)	0.0380 (5)
H8A	0.1588	−0.0464	0.6825	0.046*
H8B	0.1676	0.1110	0.6102	0.046*
C9	0.3517 (2)	−0.0332 (4)	0.65187 (14)	0.0450 (6)
N1	0.21295 (15)	0.2051 (3)	0.80041 (10)	0.0338 (4)
O1	−0.01285 (13)	0.3786 (2)	0.70850 (9)	0.0445 (4)
H1	0.1320 (13)	0.137 (3)	0.7984 (13)	0.039 (6)*
O2	0.11830 (16)	0.5682 (3)	0.63616 (10)	0.0505 (4)
O3	0.45737 (16)	0.0721 (3)	0.66196 (12)	0.0654 (6)
O4	0.34903 (16)	−0.2428 (3)	0.62772 (12)	0.0605 (5)
H4	0.2710 (17)	−0.298 (5)	0.6272 (19)	0.091*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0414 (11)	0.0339 (12)	0.0483 (13)	−0.0003 (9)	0.0073 (9)	−0.0037 (10)
C2	0.0614 (14)	0.0503 (14)	0.0444 (13)	−0.0025 (11)	0.0113 (11)	−0.0060 (11)
C3	0.0712 (16)	0.0597 (17)	0.0442 (14)	−0.0016 (13)	−0.0002 (12)	0.0022 (12)
C4	0.0599 (14)	0.0508 (15)	0.0493 (14)	0.0055 (12)	0.0018 (11)	0.0083 (12)
C5	0.0354 (10)	0.0402 (13)	0.0501 (13)	0.0051 (9)	0.0041 (9)	0.0031 (10)
C6	0.0394 (10)	0.0315 (12)	0.0404 (12)	0.0015 (8)	0.0080 (9)	−0.0046 (9)
C7	0.0291 (9)	0.0343 (11)	0.0417 (11)	−0.0007 (8)	0.0117 (8)	0.0031 (9)

C8	0.0362 (10)	0.0388 (12)	0.0406 (11)	0.0061 (8)	0.0112 (8)	0.0004 (9)
C9	0.0431 (11)	0.0461 (14)	0.0500 (13)	0.0084 (10)	0.0211 (10)	0.0042 (11)
N1	0.0291 (8)	0.0333 (10)	0.0399 (9)	−0.0015 (7)	0.0082 (7)	0.0005 (7)
O1	0.0331 (7)	0.0460 (10)	0.0559 (10)	0.0063 (6)	0.0112 (7)	0.0024 (7)
O2	0.0545 (9)	0.0429 (10)	0.0549 (10)	0.0052 (7)	0.0105 (7)	0.0122 (8)
O3	0.0414 (9)	0.0641 (12)	0.0967 (15)	0.0007 (8)	0.0303 (9)	−0.0062 (10)
O4	0.0533 (10)	0.0460 (11)	0.0875 (13)	0.0113 (8)	0.0282 (9)	−0.0067 (9)

Geometric parameters (Å, º)

C1—N1	1.503 (3)	C5—H5B	0.9700
C1—C2	1.507 (3)	C6—O1	1.239 (2)
C1—H1A	0.9700	C6—O2	1.245 (2)
C1—H1B	0.9700	C6—C7	1.544 (3)
C2—C3	1.513 (3)	C7—N1	1.503 (2)
C2—H2A	0.9700	C7—C8	1.525 (3)
C2—H2B	0.9700	C7—H7	0.9800
C3—C4	1.509 (3)	C8—C9	1.513 (3)
C3—H3A	0.9700	C8—H8A	0.9700
C3—H3B	0.9700	C8—H8B	0.9700
C4—C5	1.513 (3)	C9—O3	1.206 (3)
C4—H4A	0.9700	C9—O4	1.317 (3)
C4—H4B	0.9700	N1—H1	0.891 (9)
C5—N1	1.507 (3)	O4—H4	0.834 (10)
C5—H5A	0.9700		
N1—C1—C2	111.08 (18)	C4—C5—H5B	109.5
N1—C1—H1A	109.4	H5A—C5—H5B	108.1
C2—C1—H1A	109.4	O1—C6—O2	126.62 (19)
N1—C1—H1B	109.4	O1—C6—C7	116.74 (18)
C2—C1—H1B	109.4	O2—C6—C7	116.51 (16)
H1A—C1—H1B	108.0	N1—C7—C8	111.65 (16)
C1—C2—C3	110.87 (19)	N1—C7—C6	109.60 (14)
C1—C2—H2A	109.5	C8—C7—C6	106.99 (17)
C3—C2—H2A	109.5	N1—C7—H7	109.5
C1—C2—H2B	109.5	C8—C7—H7	109.5
C3—C2—H2B	109.5	C6—C7—H7	109.5
H2A—C2—H2B	108.1	C9—C8—C7	115.00 (18)
C4—C3—C2	109.4 (2)	C9—C8—H8A	108.5
C4—C3—H3A	109.8	C7—C8—H8A	108.5
C2—C3—H3A	109.8	C9—C8—H8B	108.5
C4—C3—H3B	109.8	C7—C8—H8B	108.5
C2—C3—H3B	109.8	H8A—C8—H8B	107.5
H3A—C3—H3B	108.3	O3—C9—O4	121.26 (19)
C3—C4—C5	111.5 (2)	O3—C9—C8	122.8 (2)
C3—C4—H4A	109.3	O4—C9—C8	115.82 (19)
C5—C4—H4A	109.3	C1—N1—C7	110.55 (15)
C3—C4—H4B	109.3	C1—N1—C5	110.28 (16)

C5—C4—H4B	109.3	C7—N1—C5	112.41 (14)
H4A—C4—H4B	108.0	C1—N1—H1	110.3 (14)
N1—C5—C4	110.80 (17)	C7—N1—H1	104.6 (14)
N1—C5—H5A	109.5	C5—N1—H1	108.6 (14)
C4—C5—H5A	109.5	C9—O4—H4	111 (2)
N1—C5—H5B	109.5		

N1—C1—C2—C3	58.1 (2)	C7—C8—C9—O3	−24.1 (3)
C1—C2—C3—C4	−57.2 (3)	C7—C8—C9—O4	158.87 (19)
C2—C3—C4—C5	56.8 (3)	C2—C1—N1—C7	178.09 (16)
C3—C4—C5—N1	−56.9 (3)	C2—C1—N1—C5	−57.0 (2)
O1—C6—C7—N1	−36.0 (2)	C8—C7—N1—C1	−179.20 (14)
O2—C6—C7—N1	147.90 (18)	C6—C7—N1—C1	−60.8 (2)
O1—C6—C7—C8	85.2 (2)	C8—C7—N1—C5	57.1 (2)
O2—C6—C7—C8	−90.9 (2)	C6—C7—N1—C5	175.46 (16)
N1—C7—C8—C9	−91.2 (2)	C4—C5—N1—C1	56.1 (2)
C6—C7—C8—C9	148.93 (18)	C4—C5—N1—C7	179.93 (17)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1	0.89 (1)	2.42 (2)	2.736 (2)	101 (2)
C1—H1*A*···O1	0.97	2.56	3.107 (3)	116
C7—H7···O3	0.98	2.48	2.879 (2)	104
N1—H1···O1^{i}	0.89 (1)	1.93 (1)	2.759 (2)	154 (2)
O4—H4···O2^{ii}	0.83 (1)	1.73 (1)	2.557 (2)	173 (3)
C1—H1*A*···O1^{iii}	0.97	2.60	3.528 (3)	160
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Symmetry codes: (i) −*x*, *y*−1/2, −*z*+3/2; (ii) *x*, *y*−1, *z*; (iii) −*x*, *y*+1/2, −*z*+3/2; (iv) −*x*+1, *y*+1/2, −*z*+3/2.