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tert-Butyl 4-formyl-1*H*-imidazole-1-carboxylate

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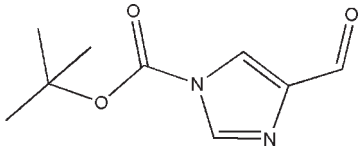
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.062; wR factor = 0.149; data-to-parameter ratio = 13.6.

In the crystal structure of the title compound, $C_9H_{12}N_2O_3$, weak intermolecular C—H···O hydrogen bonds link the molecules into chains. Further weak C—H···O hydrogen bonds together with π–π interactions [centroid–centroid distance = 3.672 (4) Å] between neighbouring chains lead to a double-chain structure propagating in [100].

Related literature

For uses of imidazole direvatives, see: Matuszak *et al.* (1976), Verras *et al.* (2004). For the synthesis of the title compound, see: Metobo *et al.* (2006).



Experimental

Crystal data

$C_9H_{12}N_2O_3$
M_r = 196.21
Triclinic, $P\overline{1}$
a = 5.972 (3) Å
b = 7.173 (7) Å
c = 12.164 (11) Å
α = 79.630 (16)°
β = 86.620 (15)°
γ = 89.326 (15)°
V = 511.7 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 K
0.14 × 0.11 × 0.03 mm

Data collection

Bruker APEX CCD area detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.987, T_{max} = 0.997
2633 measured reflections
1769 independent reflections
915 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.149
S = 0.99
1769 reflections
130 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O3^{i}	0.93	2.36	3.251 (5)	160
C9—H9C···O1^{ii}	0.96	2.65	3.531 (5)	153

Symmetry codes: (i) $x+1, y, z$; (ii) $-x+1, -y+1, -z+1$.

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT-Plus* (Bruker, 2007); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2164).

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supporting information

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S1. Comment

Imidazole derivatives are very useful compounds (Matuszak *et al.*, 1976; Verras *et al.*, 2004), and herein we report on the molecular and crystal structure of the title compound, illustrated in Fig. 1.

In the crystal packing of the title compound (Fig. 2), C2—H2···O3 hydrogen bonds involving adjacent molecules lead to the formation of a one-dimensional chain structure. Moverover, via weak C9—H9C···O1 hydrogen bonds and π-π interactions involving two neighbouring chains [the nearest atom-to-atom distance between neighbouring imidazole rings is 3.405 (5) Å], a tubular polymer structure, propagating in [100], is formed.

S2. Experimental

The title compund was synthesized according to the reported procedure (Metobo *et al.*, 2006). Colourless plate-like crystals, suitable for X-ray diffraction, were obtained by slow evaporation of a solution of the title compound in Diethyl ether at room temperature.

S3. Refinement

H atoms were placed geometrically and refined as riding atoms: C—H = 0.96 Å (CH_3) and 0.93 Å (CH), with U_{iso}(H) = k × U_{eq}(C), where k = 1.5 for (CH_3), and = 1.2 for (CH) H-atoms.

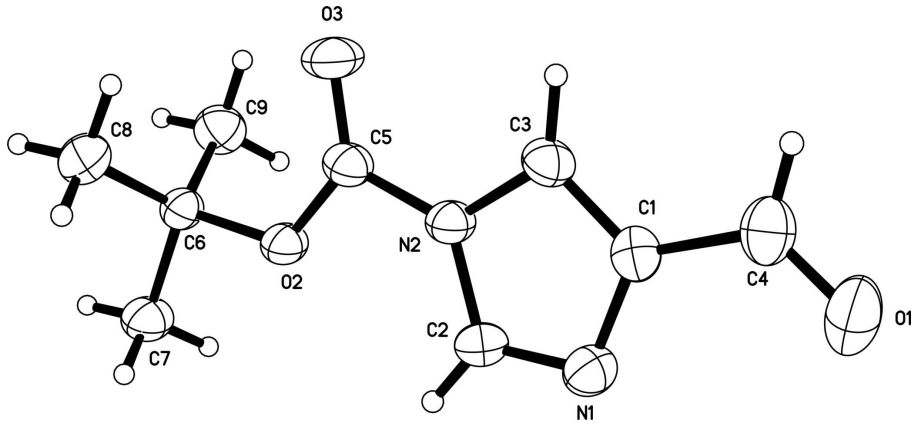

Figure 1

A view of the molecular structure of the title compound, with the atom-labeling scheme and 30% probability displacement ellipsoids.

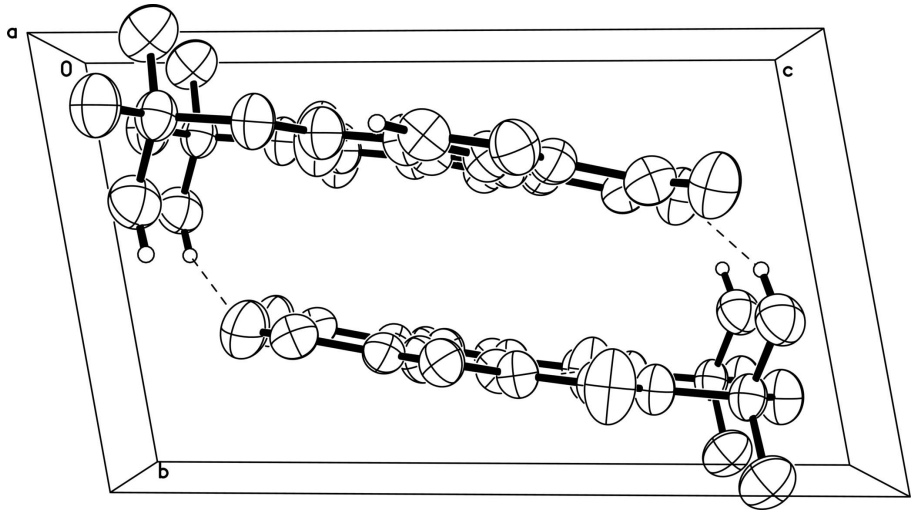

Figure 2

Perspective view along the a-axis of the crystal packing of the title compound, showing the C-H···O interactions as dashed lines [H-atoms not involved in the motif shown have been omitted for clarity].

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$\gamma = 89.326\ (15)°$
$V = 511.7\ (8)$ Å^3
$Z = 2$
$F(000) = 208$
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Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 360 reflections
$\mu = 0.10$ mm^{-1}
$T = 293$ K
Plate, colourless
0.14 × 0.11 × 0.03 mm

Data collection

Bruker APEX CCD area detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.987$, $T_{max} = 0.997$
2633 measured reflections
1769 independent reflections
915 reflections with $I > 2\sigma(I)$
$R_{int} = 0.022$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.7°$
$h = -7\rightarrow7$
$k = -8\rightarrow8$
$l = -14\rightarrow8$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.062$
$wR(F^2) = 0.149$
$S = 0.99$
1769 reflections
130 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0655P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ 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 $F^2 > \sigma(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.3982 (5)	0.3453 (4)	0.8094 (2)	0.0910 (9)
O2	0.3540 (3)	0.2118 (3)	0.27957 (17)	0.0501 (6)
O3	−0.0065 (4)	0.2329 (4)	0.34612 (19)	0.0794 (9)
N1	0.5369 (4)	0.2729 (4)	0.5822 (2)	0.0562 (8)
N2	0.2860 (4)	0.2475 (4)	0.4569 (2)	0.0480 (7)
C1	0.3197 (5)	0.2938 (4)	0.6277 (3)	0.0505 (9)
C2	0.5087 (5)	0.2466 (4)	0.4808 (3)	0.0503 (9)
H2	0.6262	0.2289	0.4301	0.060*
C3	0.1660 (5)	0.2779 (4)	0.5522 (3)	0.0529 (9)
H3	0.0110	0.2859	0.5627	0.063*
C4	0.2649 (7)	0.3323 (5)	0.7404 (3)	0.0668 (11)
H4	0.1142	0.3480	0.7606	0.080*
C5	0.1920 (6)	0.2290 (5)	0.3551 (3)	0.0519 (9)
C6	0.3044 (5)	0.1971 (5)	0.1619 (3)	0.0470 (8)
C7	0.5376 (5)	0.1878 (5)	0.1061 (3)	0.0634 (10)
H7A	0.6202	0.2993	0.1119	0.095*
H7B	0.5257	0.1806	0.0286	0.095*
H7C	0.6144	0.0775	0.1426	0.095*
C8	0.1737 (5)	0.0162 (5)	0.1638 (3)	0.0702 (11)
H8A	0.2552	−0.0899	0.2017	0.105*
H8B	0.1532	−0.0001	0.0884	0.105*
H8C	0.0299	0.0243	0.2023	0.105*
C9	0.1821 (5)	0.3734 (5)	0.1092 (3)	0.0662 (11)
H9A	0.0359	0.3771	0.1460	0.099*
H9B	0.1674	0.3714	0.0312	0.099*
H9C	0.2654	0.4835	0.1168	0.099*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.117 (2)	0.095 (2)	0.0680 (19)	−0.0003 (17)	−0.0229 (17)	−0.0287 (16)
O2	0.0374 (12)	0.0691 (16)	0.0448 (14)	−0.0015 (10)	0.0004 (10)	−0.0143 (12)

O3	0.0360 (14)	0.139 (3)	0.0686 (18)	0.0020 (13)	−0.0019 (12)	−0.0330 (17)
N1	0.0523 (18)	0.064 (2)	0.0522 (19)	−0.0018 (13)	−0.0066 (14)	−0.0074 (15)
N2	0.0376 (15)	0.0592 (19)	0.0468 (18)	−0.0004 (12)	−0.0004 (14)	−0.0089 (14)
C1	0.057 (2)	0.046 (2)	0.049 (2)	−0.0062 (16)	0.0026 (18)	−0.0079 (17)
C2	0.0387 (18)	0.055 (2)	0.055 (2)	−0.0014 (15)	−0.0029 (16)	−0.0051 (19)
C3	0.0437 (19)	0.060 (2)	0.054 (2)	−0.0038 (16)	0.0089 (18)	−0.0105 (19)
C4	0.085 (3)	0.054 (3)	0.062 (3)	−0.007 (2)	−0.005 (2)	−0.013 (2)
C5	0.040 (2)	0.064 (2)	0.051 (2)	−0.0007 (16)	0.0038 (18)	−0.0114 (18)
C6	0.0434 (18)	0.058 (2)	0.041 (2)	0.0034 (16)	−0.0065 (15)	−0.0121 (17)
C7	0.047 (2)	0.086 (3)	0.057 (2)	−0.0012 (18)	0.0030 (17)	−0.016 (2)
C8	0.055 (2)	0.074 (3)	0.086 (3)	−0.0117 (19)	−0.0017 (19)	−0.026 (2)
C9	0.067 (2)	0.068 (3)	0.063 (3)	0.0089 (19)	−0.0101 (19)	−0.007 (2)

Geometric parameters (Å, º)

O1—C4	1.206 (4)	C4—H4	0.9300
O2—C5	1.315 (4)	C6—C9	1.512 (4)
O2—C6	1.501 (4)	C6—C8	1.518 (5)
O3—C5	1.196 (3)	C6—C7	1.519 (4)
N1—C2	1.301 (4)	C7—H7A	0.9600
N1—C1	1.398 (4)	C7—H7B	0.9600
N2—C3	1.376 (4)	C7—H7C	0.9600
N2—C2	1.378 (4)	C8—H8A	0.9600
N2—C5	1.417 (4)	C8—H8B	0.9600
C1—C3	1.356 (4)	C8—H8C	0.9600
C1—C4	1.464 (5)	C9—H9A	0.9600
C2—H2	0.9300	C9—H9B	0.9600
C3—H3	0.9300	C9—H9C	0.9600
C5—O2—C6	121.3 (2)	C9—C6—C8	113.1 (3)
C2—N1—C1	104.5 (3)	O2—C6—C7	102.4 (2)
C3—N2—C2	106.1 (3)	C9—C6—C7	110.8 (3)
C3—N2—C5	125.2 (3)	C8—C6—C7	111.5 (3)
C2—N2—C5	128.7 (3)	C6—C7—H7A	109.5
C3—C1—N1	110.6 (3)	C6—C7—H7B	109.5
C3—C1—C4	124.5 (3)	H7A—C7—H7B	109.5
N1—C1—C4	124.9 (3)	C6—C7—H7C	109.5
N1—C2—N2	112.7 (3)	H7A—C7—H7C	109.5
N1—C2—H2	123.6	H7B—C7—H7C	109.5
N2—C2—H2	123.6	C6—C8—H8A	109.5
C1—C3—N2	106.1 (3)	C6—C8—H8B	109.5
C1—C3—H3	126.9	H8A—C8—H8B	109.5
N2—C3—H3	126.9	C6—C8—H8C	109.5
O1—C4—C1	125.7 (4)	H8A—C8—H8C	109.5
O1—C4—H4	117.2	H8B—C8—H8C	109.5
C1—C4—H4	117.2	C6—C9—H9A	109.5
O3—C5—O2	129.1 (3)	C6—C9—H9B	109.5
O3—C5—N2	121.5 (3)	H9A—C9—H9B	109.5

O2—C5—N2	109.4 (3)	C6—C9—H9C	109.5
O2—C6—C9	109.5 (2)	H9A—C9—H9C	109.5
O2—C6—C8	109.0 (3)	H9B—C9—H9C	109.5

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O3^{i}	0.93	2.36	3.251 (5)	160
C9—H9*C*···O1^{ii}	0.96	2.65	3.531 (5)	153

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) −*x*+1, −*y*+1, −*z*+1.