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2-Phenyl-*N*′-(2-phenylacetyl)acetohydrazide

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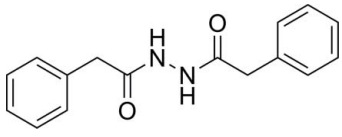
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.134; data-to-parameter ratio = 14.1.

In the title compound, $C_{16}H_{16}N_2O_2$, the N'-acetylacetohydrazide group is approximately planar (r.m.s. deviation = 0.018 Å for the eight non-H atoms) and makes dihedral angles of 81.92 (6) and 65.19 (6)° with the terminal phenyl rings. The phenyl rings form a dihedral angle of 62.60 (7)°. In the crystal, molecules are linked into sheets lying parallel to (001) by N—H···O and C—H···O hydrogen bonds. One O atom accepts one N—H···O and one C—H···O hydrogen bond and the other O atom accepts one N—H···O and two C—H···O hydrogen bonds. The N—H···O hydrogen bonds lead to $R_2^2(8)$ loops and the C—H···O hydrogen bonds generate $R_2^1(6)$ loops.

Related literature

For general background to and the pharmaceutical applications of hydrazine derivatives, see: Bredihhin & Mäeorg (2008); Ragnarsson (2001); Ling *et al.* (2001). For further synthesis details, see: Magedov & Smushkevich (1991). For standard bond-length data, see: Allen *et al.* (1987). For the stability of the temperature controller used in the data collection, see Cosier & Glazer (1986). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{16}H_{16}N_2O_2$
M_r = 268.31
Triclinic, $P\overline{1}$
a = 5.4531 (6) Å
b = 7.9283 (9) Å
c = 15.1758 (17) Å
α = 94.271 (2)°
β = 92.613 (2)°
γ = 90.830 (2)°
V = 653.50 (13) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100 K
0.35 × 0.14 × 0.05 mm

Data collection

Bruker SMART APEXII DUO CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.968, T_{max} = 0.996
12991 measured reflections
3458 independent reflections
2428 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.134
S = 1.04
3458 reflections
245 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H1*N*2···O1^{i}	0.867 (16)	1.970 (16)	2.8076 (15)	162.4 (16)
C10—H10*A*···O1^{i}	0.971 (16)	2.465 (16)	3.3103 (18)	145.3 (13)
N1—H1*N*1···O2^{ii}	0.907 (16)	1.948 (16)	2.8283 (15)	163.2 (15)
C7—H7*A*···O2^{ii}	0.973 (16)	2.479 (16)	3.3209 (18)	144.8 (13)
C7—H7*B*···O2^{iii}	1.00 (2)	2.56 (2)	3.4929 (19)	155.2 (13)

Symmetry codes: (i) $-x+1, -y+1, -z$; (ii) $-x+2, -y+2, -z$; (iii) $-x+1, -y+2, -z$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6773).

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§ Thomson Reuters ResearcherID: A-3561-2009.

supplementary materials

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Comment

Hydrazine derivatives are widely used in the pharmaceutical applications and also as precursors in organic synthesis (Bredihhin & Mäeorg, 2008). Several hydrazine derivatives were shown to be effective for treatment of tuberculosis, Parkinson's disease and hypertension (Ragnarsson, 2001). Moreover, some hydrazines possess neuroprotective activity and are used as antidepressant drugs (Ling *et al.*, 2001).

In the title compound, Fig. 1, the *N*′-acetylacetohydrazide moiety (O1/O2/N1/N2/C7-C10) is approximately planar (r.m.s. deviation = 0.018 Å for the 8 non-H atoms) and makes dihedral angles of 81.92 (6) and 65.19 (6)° with the two terminal benzene rings (C1-C6 and C11-C16), respectively. The two benzene rings form a dihedral angle of 62.60 (7)°. Bond lengths (Allen *et al.*, 1987) and angles are within normal ranges.

In the crystal (Fig.2), molecules are linked into planes parallel to the (001) *via* intermolecular N1–H1N1···O2, C7–H7A···O2 and C7–H7B···O2 trifurcated acceptor bonds (Table 1) and N2–H1N2···O1 and C10–H10A···O1 bifurcated acceptor bonds (Table 1), generating $R_2^1(6)$ ring motifs (Bernstein *et al.*, 1995).

Experimental

The title compound was prepared by the reaction of 2-phenylacetyl chloride with 2-phenylacetohydrazide in the presence of sodium carbonate in water at 5-10 °C (Magedov & Smushkevich, 1991).

Refinement

All H atoms were located in a difference Fourier map and refined freely with N–H = 0.869 (18)-0.908 (19) Å and C–H = 0.942 (19)-1.013 (18) Å.

Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

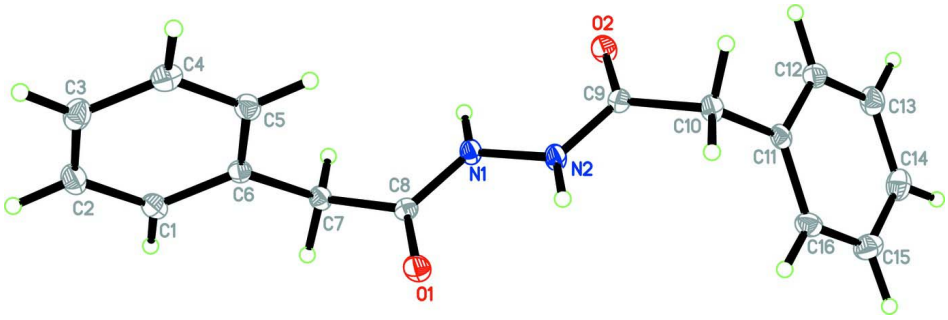

Figure 1

The molecular structure of the title compound showing 50% probability displacement ellipsoids for non-H atoms.

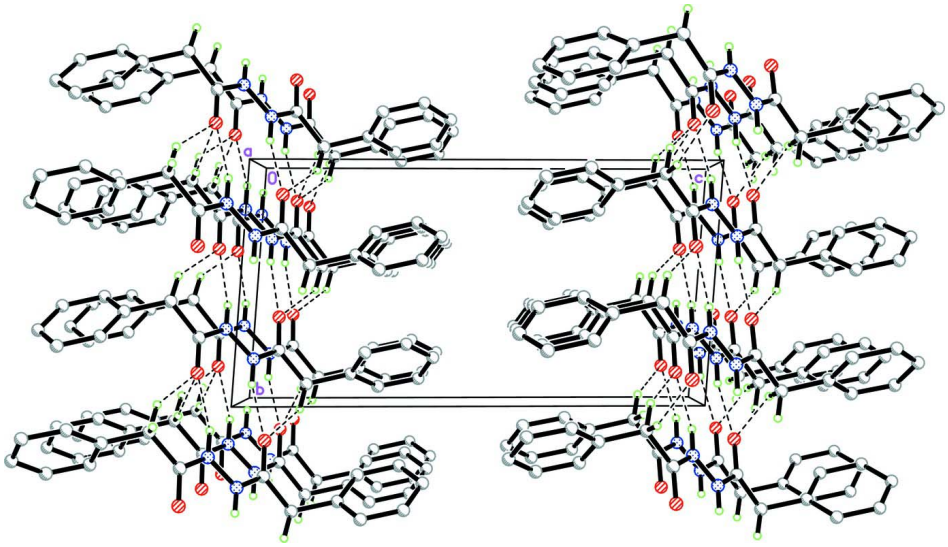

Figure 2

The crystal structure of the title compound, viewed along the *a* axis. H atoms not involved in hydrogen bonds (dashed lines) have been omitted for clarity.

2-Phenyl-*N*′-(2-phenylacetyl)acetohydrazide

Crystal data

$C_{16}H_{16}N_2O_2$
$M_r = 268.31$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 5.4531\ (6)$ Å
$b = 7.9283\ (9)$ Å
$c = 15.1758\ (17)$ Å
$\alpha = 94.271\ (2)°$
$\beta = 92.613\ (2)°$
$\gamma = 90.830\ (2)°$
$V = 653.50\ (13)$ Å^3
$Z = 2$
$F(000) = 284$
$D_x = 1.364$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3410 reflections
$\theta = 4.0–30.0°$
$\mu = 0.09$ mm^{-1}
$T = 100$ K
Needle, colourless
0.35 × 0.14 × 0.05 mm

Data collection

Bruker SMART APEXII DUO CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.968, T_{max} = 0.996
12991 measured reflections
3458 independent reflections
2428 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 29.0°, θ_{min} = 1.4°
$h = -7 \rightarrow 7$
$k = -10 \rightarrow 10$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.134
S = 1.04
3458 reflections
245 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
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0709P)^2 + 0.1901P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

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 $F^2 > 2$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}
O1	0.40065 (18)	0.64320 (12)	0.06665 (6)	0.0165 (2)
O2	1.08994 (18)	0.85895 (12)	−0.07188 (6)	0.0166 (2)
N1	0.7067 (2)	0.81353 (14)	0.02864 (7)	0.0131 (2)
N2	0.7869 (2)	0.68791 (14)	−0.03185 (7)	0.0136 (2)
C1	0.2796 (3)	0.94134 (17)	0.29275 (9)	0.0154 (3)
C2	0.3026 (3)	0.90738 (18)	0.38118 (9)	0.0185 (3)
C3	0.4978 (3)	0.81340 (18)	0.41175 (9)	0.0184 (3)
C4	0.6710 (3)	0.75379 (18)	0.35344 (9)	0.0180 (3)
C5	0.6502 (2)	0.78955 (17)	0.26515 (9)	0.0153 (3)
C6	0.4540 (2)	0.88282 (16)	0.23362 (8)	0.0127 (3)
C7	0.4336 (3)	0.92581 (17)	0.13786 (8)	0.0129 (3)
C8	0.5093 (2)	0.78171 (16)	0.07486 (8)	0.0120 (3)
C9	0.9839 (2)	0.71983 (16)	−0.07846 (8)	0.0120 (3)
C10	1.0630 (3)	0.57244 (17)	−0.13972 (8)	0.0137 (3)
C11	1.0445 (2)	0.61346 (16)	−0.23584 (8)	0.0127 (3)

C12	1.2278 (3)	0.70965 (18)	−0.27062 (9)	0.0162 (3)
C13	1.2100 (3)	0.74792 (18)	−0.35846 (9)	0.0186 (3)
C14	1.0109 (3)	0.68811 (19)	−0.41296 (9)	0.0200 (3)
C15	0.8286 (3)	0.59203 (19)	−0.37894 (9)	0.0196 (3)
C16	0.8446 (3)	0.55437 (17)	−0.29055 (9)	0.0161 (3)
H1N1	0.787 (3)	0.915 (2)	0.0321 (11)	0.023 (5)*
H1N2	0.705 (3)	0.593 (2)	−0.0350 (11)	0.017 (4)*
H1A	0.148 (3)	1.007 (2)	0.2720 (11)	0.022 (4)*
H2A	0.175 (3)	0.951 (2)	0.4219 (10)	0.017 (4)*
H3A	0.519 (4)	0.786 (2)	0.4710 (13)	0.031 (5)*
H4A	0.809 (3)	0.686 (2)	0.3727 (11)	0.021 (4)*
H5A	0.775 (3)	0.747 (2)	0.2245 (11)	0.018 (4)*
H7A	0.529 (3)	1.028 (2)	0.1304 (10)	0.018 (4)*
H7B	0.259 (4)	0.953 (2)	0.1223 (12)	0.027 (5)*
H10A	0.967 (3)	0.471 (2)	−0.1318 (10)	0.016 (4)*
H10B	1.240 (3)	0.554 (2)	−0.1200 (11)	0.021 (4)*
H12A	1.373 (3)	0.757 (2)	−0.2322 (11)	0.022 (4)*
H13A	1.339 (3)	0.814 (2)	−0.3815 (12)	0.029 (5)*
H14A	1.002 (3)	0.713 (2)	−0.4733 (12)	0.028 (5)*
H16A	0.720 (3)	0.489 (2)	−0.2662 (12)	0.029 (5)*
H15A	0.692 (3)	0.549 (2)	−0.4190 (11)	0.017 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0172 (5)	0.0123 (5)	0.0198 (5)	−0.0052 (4)	0.0047 (4)	−0.0010 (4)
O2	0.0172 (5)	0.0119 (5)	0.0206 (5)	−0.0033 (4)	0.0051 (4)	−0.0013 (4)
N1	0.0151 (6)	0.0101 (5)	0.0141 (5)	−0.0019 (4)	0.0042 (4)	−0.0016 (4)
N2	0.0156 (6)	0.0100 (5)	0.0150 (5)	−0.0023 (4)	0.0052 (4)	−0.0021 (4)
C1	0.0137 (6)	0.0143 (6)	0.0184 (6)	−0.0001 (5)	0.0029 (5)	0.0002 (5)
C2	0.0195 (7)	0.0175 (7)	0.0185 (7)	−0.0024 (5)	0.0059 (5)	−0.0006 (5)
C3	0.0235 (8)	0.0176 (7)	0.0143 (6)	−0.0031 (6)	0.0014 (5)	0.0021 (5)
C4	0.0170 (7)	0.0173 (7)	0.0191 (7)	0.0005 (5)	−0.0028 (5)	0.0005 (5)
C5	0.0142 (6)	0.0146 (6)	0.0169 (6)	0.0002 (5)	0.0022 (5)	−0.0011 (5)
C6	0.0128 (6)	0.0107 (6)	0.0143 (6)	−0.0038 (5)	0.0017 (5)	−0.0007 (5)
C7	0.0139 (6)	0.0106 (6)	0.0143 (6)	0.0000 (5)	0.0028 (5)	−0.0003 (5)
C8	0.0124 (6)	0.0114 (6)	0.0121 (6)	−0.0005 (5)	−0.0006 (5)	0.0013 (4)
C9	0.0134 (6)	0.0112 (6)	0.0115 (6)	−0.0001 (5)	0.0012 (5)	0.0013 (4)
C10	0.0156 (7)	0.0107 (6)	0.0149 (6)	−0.0003 (5)	0.0039 (5)	0.0007 (5)
C11	0.0132 (6)	0.0090 (6)	0.0161 (6)	0.0016 (5)	0.0037 (5)	−0.0008 (5)
C12	0.0148 (7)	0.0155 (6)	0.0179 (6)	−0.0020 (5)	0.0026 (5)	−0.0013 (5)
C13	0.0211 (7)	0.0169 (7)	0.0182 (7)	−0.0019 (5)	0.0060 (5)	0.0009 (5)
C14	0.0254 (8)	0.0191 (7)	0.0155 (6)	0.0040 (6)	0.0016 (6)	0.0016 (5)
C15	0.0185 (7)	0.0185 (7)	0.0210 (7)	0.0010 (6)	−0.0043 (6)	−0.0005 (5)
C16	0.0131 (6)	0.0140 (6)	0.0212 (7)	−0.0018 (5)	0.0020 (5)	0.0012 (5)

Geometric parameters (Å, º)

O1—C8	1.2355 (16)	C7—C8	1.5089 (18)
O2—C9	1.2332 (16)	C7—H7A	0.975 (18)

N1—C8	1.3426 (16)	C7—H7B	1.002 (19)
N1—N2	1.3922 (14)	C9—C10	1.5183 (18)
N1—H1N1	0.908 (19)	C10—C11	1.5172 (18)
N2—C9	1.3443 (16)	C10—H10A	0.972 (17)
N2—H1N2	0.869 (18)	C10—H10B	1.013 (18)
C1—C2	1.3888 (19)	C11—C16	1.3934 (19)
C1—C6	1.3977 (18)	C11—C12	1.3951 (18)
C1—H1A	0.950 (18)	C12—C13	1.3884 (19)
C2—C3	1.390 (2)	C12—H12A	1.009 (18)
C2—H2A	1.000 (16)	C13—C14	1.390 (2)
C3—C4	1.388 (2)	C13—H13A	0.963 (19)
C3—H3A	0.942 (19)	C14—C15	1.385 (2)
C4—C5	1.3899 (19)	C14—H14A	0.949 (18)
C4—H4A	0.977 (17)	C15—C16	1.3948 (19)
C5—C6	1.3960 (18)	C15—H15A	0.980 (17)
C5—H5A	0.986 (17)	C16—H16A	0.954 (19)
C6—C7	1.5167 (18)		

C8—N1—N2	118.83 (11)	O1—C8—N1	121.88 (12)
C8—N1—H1N1	123.8 (11)	O1—C8—C7	122.94 (12)
N2—N1—H1N1	117.2 (11)	N1—C8—C7	115.18 (11)
C9—N2—N1	118.90 (11)	O2—C9—N2	122.08 (12)
C9—N2—H1N2	125.2 (11)	O2—C9—C10	123.08 (12)
N1—N2—H1N2	115.9 (11)	N2—C9—C10	114.84 (11)
C2—C1—C6	120.35 (13)	C11—C10—C9	111.62 (11)
C2—C1—H1A	120.4 (10)	C11—C10—H10A	110.1 (9)
C6—C1—H1A	119.2 (10)	C9—C10—H10A	111.1 (10)
C1—C2—C3	120.42 (13)	C11—C10—H10B	110.7 (10)
C1—C2—H2A	118.5 (9)	C9—C10—H10B	104.3 (10)
C3—C2—H2A	121.0 (9)	H10A—C10—H10B	108.8 (14)
C4—C3—C2	119.67 (13)	C16—C11—C12	119.24 (12)
C4—C3—H3A	117.1 (12)	C16—C11—C10	120.29 (12)
C2—C3—H3A	123.2 (12)	C12—C11—C10	120.47 (12)
C3—C4—C5	120.00 (13)	C13—C12—C11	120.42 (14)
C3—C4—H4A	121.6 (10)	C13—C12—H12A	118.5 (10)
C5—C4—H4A	118.4 (10)	C11—C12—H12A	121.0 (10)
C4—C5—C6	120.81 (12)	C12—C13—C14	120.18 (13)
C4—C5—H5A	119.2 (9)	C12—C13—H13A	119.3 (11)
C6—C5—H5A	120.0 (9)	C14—C13—H13A	120.5 (11)
C5—C6—C1	118.74 (12)	C15—C14—C13	119.70 (13)
C5—C6—C7	121.05 (11)	C15—C14—H14A	120.6 (12)
C1—C6—C7	120.17 (12)	C13—C14—H14A	119.7 (12)
C8—C7—C6	112.43 (11)	C14—C15—C16	120.35 (14)
C8—C7—H7A	111.1 (10)	C14—C15—H15A	118.1 (10)
C6—C7—H7A	110.0 (9)	C16—C15—H15A	121.5 (10)
C8—C7—H7B	108.1 (11)	C11—C16—C15	120.10 (13)
C6—C7—H7B	108.9 (10)	C11—C16—H16A	118.7 (11)
H7A—C7—H7B	105.9 (14)	C15—C16—H16A	121.2 (11)

C8—N1—N2—C9	179.72 (11)	N1—N2—C9—O2	−2.93 (19)
C6—C1—C2—C3	−0.6 (2)	N1—N2—C9—C10	177.53 (11)
C1—C2—C3—C4	0.2 (2)	O2—C9—C10—C11	−61.91 (17)
C2—C3—C4—C5	0.6 (2)	N2—C9—C10—C11	117.63 (13)
C3—C4—C5—C6	−1.1 (2)	C9—C10—C11—C16	−100.39 (15)
C4—C5—C6—C1	0.6 (2)	C9—C10—C11—C12	80.05 (15)
C4—C5—C6—C7	178.53 (13)	C16—C11—C12—C13	0.8 (2)
C2—C1—C6—C5	0.2 (2)	C10—C11—C12—C13	−179.64 (12)
C2—C1—C6—C7	−177.69 (13)	C11—C12—C13—C14	−1.1 (2)
C5—C6—C7—C8	39.28 (18)	C12—C13—C14—C15	0.9 (2)
C1—C6—C7—C8	−142.87 (13)	C13—C14—C15—C16	−0.3 (2)
N2—N1—C8—O1	1.69 (19)	C12—C11—C16—C15	−0.3 (2)
N2—N1—C8—C7	−179.17 (11)	C10—C11—C16—C15	−179.84 (12)
C6—C7—C8—O1	62.54 (17)	C14—C15—C16—C11	0.1 (2)
C6—C7—C8—N1	−116.59 (13)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H1*N*2···O1^{i}	0.867 (16)	1.970 (16)	2.8076 (15)	162.4 (16)
C10—H10*A*···O1^{i}	0.971 (16)	2.465 (16)	3.3103 (18)	145.3 (13)
N1—H1*N*1···O2^{ii}	0.907 (16)	1.948 (16)	2.8283 (15)	163.2 (15)
C7—H7*A*···O2^{ii}	0.973 (16)	2.479 (16)	3.3209 (18)	144.8 (13)
C7—H7*B*···O2^{iii}	1.00 (2)	2.56 (2)	3.4929 (19)	155.2 (13)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*; (ii) −*x*+2, −*y*+2, −*z*; (iii) −*x*+1, −*y*+2, −*z*.