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Crystal structure of (4*Z*)-4-[(dimethylamino)methylidene]-3,5-dioxo-2-phenylpyrazolidine-1-carbaldehyde

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Crystal structure of (4*Z*)-4-[(dimethylamino)methylidene]-3,5-dioxo-2-phenylpyrazolidine-1-carbaldehyde

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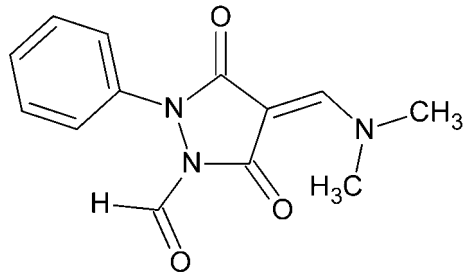
In the title compound, $C_{13}H_{13}N_3O_3$, the pyrazolidine ring adopts a shallow envelope conformation, with the carbonyl C atom closest to the benzene ring as the flap [deviation of 0.126 (1) Å from the plane through the remaining atoms (r.m.s. deviation = 0.011 Å)]. The dihedral angle between the pyrazolidine ring (all atoms) and the benzene ring is 51.09 (4)°. An extremely short (2.08 Å) intramolecular C—H···O contact is seen. In the crystal, molecules are linked by C—H···O bonds, generating [010] chains. Extremely weak C—H···π interactions are also observed.

Keywords: crystal structure; pyrazolones; short intramolecular C—H···O contact; C—H···O hydrogen bonds; C—H···π interactions.

CCDC reference: 1402532

1. Related literature

For biological studies of azole compounds, see: Patel *et al.* (2012); Vijesh *et al.* (2011). For various medicinal and industrial applications of pyrrazole-containing compounds, see: Jin *et al.* (2011); Zhang *et al.* (2010); El-Sabbagh *et al.* (2009); Dekhane *et al.* (2011); Rostom *et al.* (2003); Zhou *et al.* (2010); Finkelstein & Strock (1997).



2. Experimental

2.1. Crystal data

$C_{13}H_{13}N_3O_3$
M_r = 259.26
Monoclinic, $C2/c$
a = 26.4235 (9) Å
b = 6.1033 (2) Å
c = 16.8611 (6) Å
β = 113.272 (1)°
V = 2497.96 (15) Å^3
Z = 8
Cu $K\alpha$ radiation
μ = 0.84 mm^{-1}
T = 150 K
0.24 × 0.15 × 0.05 mm

2.2. Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Absorption correction: multi-scan (*TWINABS*; Sheldrick, 2009)
T_{min} = 0.82, T_{max} = 0.96
26486 measured reflections
4565 independent reflections
3979 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.104
S = 1.04
4565 reflections
175 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

*Cg*1 is the centroid of the C1/C2/C3/N1/N2 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6*A*···O2	0.98	2.08	3.016 (2)	160
C5—H5*C*···O3^{i}	0.98	2.52	3.1803 (19)	124
C7—H7···O2^{ii}	0.95	2.29	3.0663 (16)	139
C5—H5*B*···*Cg*1^{iii}	0.98	2.98	3.8823 (18)	153

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

Data collection: *APEX2* (Bruker, 2014); cell refinement: *SAINT* (Bruker, 2014); data reduction: *SAINT*; program(s) used to solve structure: *SHELXT* (Sheldrick, 2015*a*); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015*b*); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2012); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

Acknowledgements

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Tulane Crystallography Laboratory are gratefully acknowledged.

Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7425).

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supporting information

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Crystal structure of (4*Z*)-4-[(dimethylamino)methylidene]-3,5-dioxo-2-phenylpyrazolidine-1-carbaldehyde

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S1. Comment

Azole compounds are extensively studied and widely used as anti-microbial agents (Patel *et al.*, 2012; Vijesh *et al.*, 2011). Recently, urea derivatives of pyrazole have been reported as potent inhibitors of p38 kinase (Jin *et al.*, 2011). Many of other pyrazole scaffold compounds are reported to have broad spectra of biological activities, such as anti-fungal (Zhang *et al.*, 2010), anti-viral (El-Sabbagh *et al.*, 2009), anti-inflammatory (Dekhane *et al.*, 2011), anti-tumor, anti-HCV (Rostom *et al.*, 2003), herbicidal (Zhou *et al.*, 2010) and insecticidal activities (Finkelstein & Strock, 1997). In view of such findings and as a continuation of our study on the synthesis of potential bio-active heterocyclic molecules, we report here the synthesis and crystal structure of the title compound.

In the title compound, the pyrazolidine ring is slightly twisted with an r.m.s. deviation from the mean plane of the 5 atoms forming the ring of 0.036 Å. The dihedral angle between this plane and that of the phenyl ring is 51.09 (4)° (Fig. 1).

S2. Experimental

To phosphorous oxychloride (0.1 mol, 10 ml), in a conical flask with a magnetic stirrer, dry dimethylformamide (35 ml) was added drop-wise with stirring at 303–308 K for 30 min. Then a solution of 1-phenylpyrazolidine-3,5-dione (0.05 mol, 8.8 g) in dimethylformamide (15 ml), was added drop-wise with continuous stirring while ensuring that the temperature did not exceed 318 K. The reaction mixture was stirred overnight and poured onto crushed ice. The solid product was collected by filtration and recrystallized from ethanol to give colourless crystals in 75% yield (m. p. 453–455 K).

S3. Refinement

H-atoms were placed in calculated positions (C—H = 0.95 - 0.98 Å) and included as riding contributions with isotropic displacement parameters 1.2 - 1.5 times those of the attached carbon atoms. The model was refined as a 2-component twin.

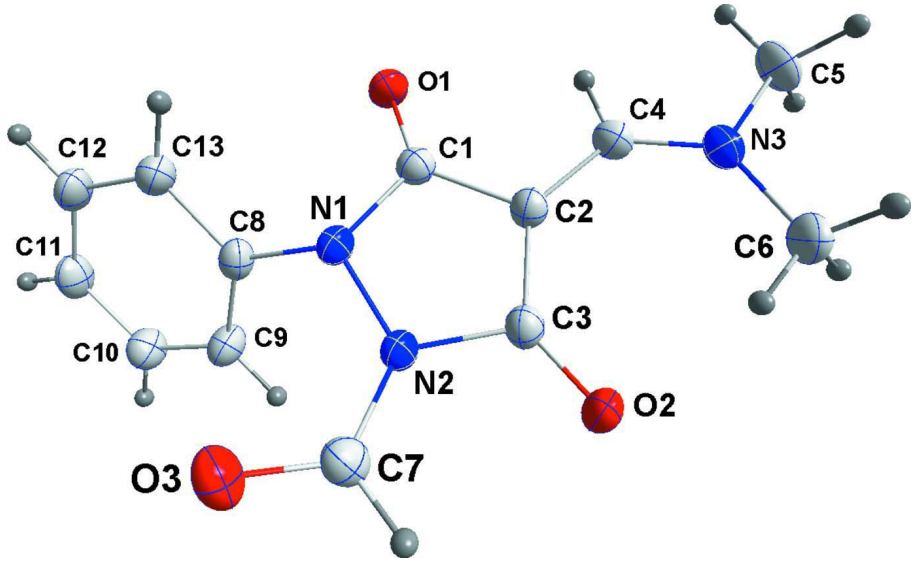

Figure 1

The title molecule with 50% probability ellipsoids.

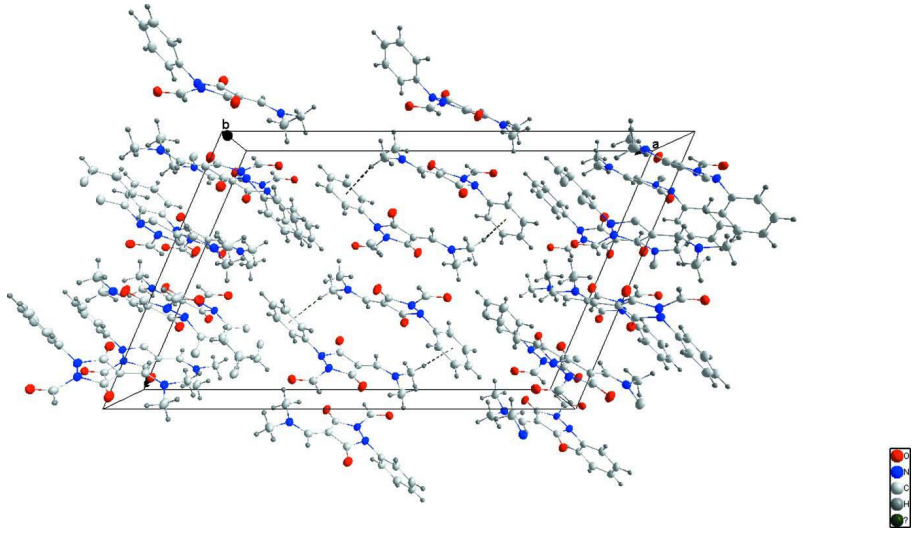

Figure 2

Packing viewed down the *b* axis. C—H···π interactions are shown by dotted lines.

(4*Z*)-4-[(Dimethylamino)methylidene]-3,5-dioxo-2-phenylpyrazolidine-1-carbaldehyde

Crystal data

$C_{13}H_{13}N_3O_3$
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$b = 6.1033\ (2)$ Å
$c = 16.8611\ (6)$ Å
$\beta = 113.272\ (1)°$
$V = 2497.96\ (15)$ Å^3
$Z = 8$
$F(000) = 1088$
$D_x = 1.379$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 9978 reflections
$\theta = 3.6–72.3°$
$\mu = 0.84$ mm^{-1}
$T = 150$ K
Rod, colourless
0.24 × 0.15 × 0.05 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC IμS micro–focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*TWINABS*; Sheldrick, 2009)
T_{min} = 0.82, T_{max} = 0.96
26486 measured reflections
4565 independent reflections
3979 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 72.3°, θ_{min} = 3.6°
h = −32→30
k = −7→7
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.104
S = 1.04
4565 reflections
175 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
$w = 1/[\sigma^2(F_o^2) + (0.0577P)^2 + 0.7347P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Special details

Experimental. Analysis of 3764 reflections having I/σ(I) > 12 and chosen from the full data set with *CELL_NOW* (Sheldrick, 2008) showed the crystal to belong to the monoclinic system and to be twinned by a 180° rotation about the *c** axis. The raw data were processed using the multi-component version of *SAINT* under control of the two-component orientation file generated by *CELL_NOW*.

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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. H-atoms were placed in calculated positions (C—H = 0.95 - 0.98 Å) and included as riding contributions with isotropic displacement parameters 1.2 - 1.5 times those of the attached carbon atoms. The model was refined as a 2-component twin.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
O1	0.43175 (4)	0.79022 (16)	0.28697 (7)	0.0296 (2)
O2	0.52891 (4)	0.15926 (16)	0.42906 (7)	0.0324 (3)
O3	0.37052 (4)	0.10698 (18)	0.39957 (6)	0.0316 (3)

N1	0.40831 (4)	0.46179 (18)	0.33205 (7)	0.0236 (3)
N2	0.43832 (4)	0.26978 (18)	0.36829 (7)	0.0239 (3)
N3	0.59876 (5)	0.64368 (19)	0.42207 (8)	0.0265 (3)
C1	0.44610 (5)	0.6170 (2)	0.32599 (8)	0.0233 (3)
C2	0.50109 (5)	0.5284 (2)	0.37179 (8)	0.0235 (3)
C3	0.49589 (5)	0.3060 (2)	0.39467 (8)	0.0242 (3)
C4	0.54556 (5)	0.6654 (2)	0.38045 (9)	0.0249 (3)
H4	0.5349	0.8001	0.3502	0.030*
C5	0.63539 (6)	0.8195 (3)	0.41755 (10)	0.0344 (3)
H5A	0.6133	0.9445	0.3861	0.052*
H5B	0.6580	0.7661	0.3874	0.052*
H5C	0.6594	0.8652	0.4761	0.052*
C6	0.62712 (6)	0.4598 (3)	0.47712 (10)	0.0344 (3)
H6A	0.6002	0.3471	0.4750	0.052*
H6B	0.6462	0.5109	0.5367	0.052*
H6C	0.6540	0.3978	0.4566	0.052*
C7	0.41757 (5)	0.1104 (2)	0.40511 (8)	0.0255 (3)
H7	0.4416	−0.0034	0.4367	0.031*
C8	0.35475 (5)	0.4373 (2)	0.26388 (8)	0.0235 (3)
C9	0.34078 (5)	0.2502 (2)	0.21315 (9)	0.0275 (3)
H9	0.3667	0.1349	0.2227	0.033*
C10	0.28831 (6)	0.2336 (3)	0.14813 (9)	0.0311 (3)
H10	0.2783	0.1062	0.1129	0.037*
C11	0.25040 (6)	0.4019 (3)	0.13433 (9)	0.0311 (3)
H11	0.2146	0.3899	0.0897	0.037*
C12	0.26490 (6)	0.5880 (2)	0.18593 (10)	0.0308 (3)
H12	0.2390	0.7031	0.1765	0.037*
C13	0.31717 (5)	0.6066 (2)	0.25127 (9)	0.0271 (3)
H13	0.3271	0.7333	0.2868	0.033*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0274 (5)	0.0239 (5)	0.0339 (5)	0.0033 (4)	0.0083 (4)	0.0053 (4)
O2	0.0221 (5)	0.0284 (5)	0.0409 (6)	0.0034 (4)	0.0063 (4)	0.0100 (4)
O3	0.0259 (5)	0.0404 (6)	0.0290 (5)	−0.0054 (4)	0.0115 (4)	0.0019 (4)
N1	0.0201 (5)	0.0227 (6)	0.0262 (6)	0.0027 (4)	0.0072 (4)	0.0031 (4)
N2	0.0190 (5)	0.0234 (6)	0.0267 (6)	0.0013 (4)	0.0062 (4)	0.0053 (4)
N3	0.0232 (5)	0.0306 (6)	0.0260 (6)	−0.0047 (4)	0.0099 (4)	−0.0026 (5)
C1	0.0241 (6)	0.0232 (6)	0.0227 (6)	0.0005 (5)	0.0093 (5)	−0.0009 (5)
C2	0.0211 (6)	0.0252 (7)	0.0233 (6)	0.0009 (5)	0.0077 (5)	0.0017 (5)
C3	0.0206 (6)	0.0268 (6)	0.0231 (6)	−0.0003 (5)	0.0063 (5)	0.0013 (5)
C4	0.0266 (6)	0.0250 (6)	0.0233 (6)	−0.0015 (5)	0.0102 (5)	−0.0005 (5)
C5	0.0296 (7)	0.0432 (8)	0.0314 (7)	−0.0132 (6)	0.0132 (6)	−0.0043 (7)
C6	0.0237 (6)	0.0348 (8)	0.0386 (8)	0.0007 (6)	0.0059 (6)	−0.0005 (6)
C7	0.0254 (6)	0.0271 (7)	0.0216 (6)	−0.0029 (5)	0.0066 (5)	0.0022 (5)
C8	0.0195 (6)	0.0289 (7)	0.0227 (6)	0.0010 (5)	0.0090 (5)	0.0033 (5)
C9	0.0247 (6)	0.0310 (7)	0.0258 (7)	0.0054 (5)	0.0089 (5)	0.0001 (5)

C10	0.0289 (7)	0.0344 (8)	0.0273 (7)	−0.0001 (6)	0.0082 (6)	−0.0029 (6)
C11	0.0212 (6)	0.0397 (8)	0.0281 (7)	0.0010 (6)	0.0053 (5)	0.0056 (6)
C12	0.0222 (6)	0.0319 (7)	0.0383 (8)	0.0060 (5)	0.0121 (6)	0.0072 (6)
C13	0.0240 (6)	0.0263 (7)	0.0326 (7)	0.0018 (5)	0.0128 (6)	0.0007 (5)

Geometric parameters (Å, º)

O1—C1	1.2234 (17)	C5—H5C	0.9800
O2—C3	1.2247 (17)	C6—H6A	0.9800
O3—C7	1.2096 (17)	C6—H6B	0.9800
N1—C1	1.4094 (17)	C6—H6C	0.9800
N1—N2	1.4116 (15)	C7—H7	0.9500
N1—C8	1.4356 (16)	C8—C9	1.387 (2)
N2—C7	1.3789 (17)	C8—C13	1.3898 (18)
N2—C3	1.4236 (16)	C9—C10	1.3903 (19)
N3—C4	1.3064 (17)	C9—H9	0.9500
N3—C6	1.4607 (19)	C10—C11	1.389 (2)
N3—C5	1.4669 (18)	C10—H10	0.9500
C1—C2	1.4538 (17)	C11—C12	1.389 (2)
C2—C4	1.4019 (18)	C11—H11	0.9500
C2—C3	1.4324 (19)	C12—C13	1.390 (2)
C4—H4	0.9500	C12—H12	0.9500
C5—H5A	0.9800	C13—H13	0.9500
C5—H5B	0.9800		
C1—N1—N2	107.25 (10)	N3—C6—H6A	109.5
C1—N1—C8	120.96 (11)	N3—C6—H6B	109.5
N2—N1—C8	117.89 (10)	H6A—C6—H6B	109.5
C7—N2—N1	121.70 (11)	N3—C6—H6C	109.5
C7—N2—C3	122.33 (11)	H6A—C6—H6C	109.5
N1—N2—C3	110.76 (10)	H6B—C6—H6C	109.5
C4—N3—C6	126.32 (12)	O3—C7—N2	123.82 (13)
C4—N3—C5	119.34 (12)	O3—C7—H7	118.1
C6—N3—C5	114.31 (12)	N2—C7—H7	118.1
O1—C1—N1	122.81 (12)	C9—C8—C13	121.19 (12)
O1—C1—C2	129.76 (12)	C9—C8—N1	121.16 (11)
N1—C1—C2	107.42 (11)	C13—C8—N1	117.64 (12)
C4—C2—C3	134.64 (12)	C8—C9—C10	119.07 (13)
C4—C2—C1	117.00 (12)	C8—C9—H9	120.5
C3—C2—C1	108.28 (11)	C10—C9—H9	120.5
O2—C3—N2	120.52 (12)	C11—C10—C9	120.43 (14)
O2—C3—C2	133.97 (12)	C11—C10—H10	119.8
N2—C3—C2	105.51 (11)	C9—C10—H10	119.8
N3—C4—C2	132.47 (13)	C10—C11—C12	119.85 (13)
N3—C4—H4	113.8	C10—C11—H11	120.1
C2—C4—H4	113.8	C12—C11—H11	120.1
N3—C5—H5A	109.5	C11—C12—C13	120.33 (13)
N3—C5—H5B	109.5	C11—C12—H12	119.8

H5A—C5—H5B	109.5	C13—C12—H12	119.8
N3—C5—H5C	109.5	C8—C13—C12	119.12 (13)
H5A—C5—H5C	109.5	C8—C13—H13	120.4
H5B—C5—H5C	109.5	C12—C13—H13	120.4
C1—N1—N2—C7	161.44 (12)	C1—C2—C3—N2	−4.26 (14)
C8—N1—N2—C7	−57.85 (16)	C6—N3—C4—C2	−2.8 (2)
C1—N1—N2—C3	6.44 (14)	C5—N3—C4—C2	179.28 (14)
C8—N1—N2—C3	147.14 (11)	C3—C2—C4—N3	−9.4 (3)
N2—N1—C1—O1	170.26 (12)	C1—C2—C4—N3	174.34 (14)
C8—N1—C1—O1	31.01 (19)	N1—N2—C7—O3	10.0 (2)
N2—N1—C1—C2	−8.87 (14)	C3—N2—C7—O3	162.12 (13)
C8—N1—C1—C2	−148.12 (11)	C1—N1—C8—C9	111.30 (15)
O1—C1—C2—C4	6.4 (2)	N2—N1—C8—C9	−23.84 (17)
N1—C1—C2—C4	−174.52 (11)	C1—N1—C8—C13	−69.53 (16)
O1—C1—C2—C3	−170.80 (13)	N2—N1—C8—C13	155.33 (12)
N1—C1—C2—C3	8.25 (14)	C13—C8—C9—C10	0.6 (2)
C7—N2—C3—O2	24.0 (2)	N1—C8—C9—C10	179.72 (13)
N1—N2—C3—O2	178.78 (12)	C8—C9—C10—C11	−0.2 (2)
C7—N2—C3—C2	−156.09 (12)	C9—C10—C11—C12	−0.2 (2)
N1—N2—C3—C2	−1.27 (14)	C10—C11—C12—C13	0.0 (2)
C4—C2—C3—O2	−0.8 (3)	C9—C8—C13—C12	−0.7 (2)
C1—C2—C3—O2	175.68 (15)	N1—C8—C13—C12	−179.87 (12)
C4—C2—C3—N2	179.21 (14)	C11—C12—C13—C8	0.4 (2)

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C1/C2/C3/N1/N2 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6*A*···O2	0.98	2.08	3.016 (2)	160
C5—H5*C*···O3^{i}	0.98	2.52	3.1803 (19)	124
C7—H7···O2^{ii}	0.95	2.29	3.0663 (16)	139
C5—H5*B*···*Cg*1^{iii}	0.98	2.98	3.8823 (18)	153

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