

# *N*-(4-Methoxy-2-nitrophenyl)acetamide

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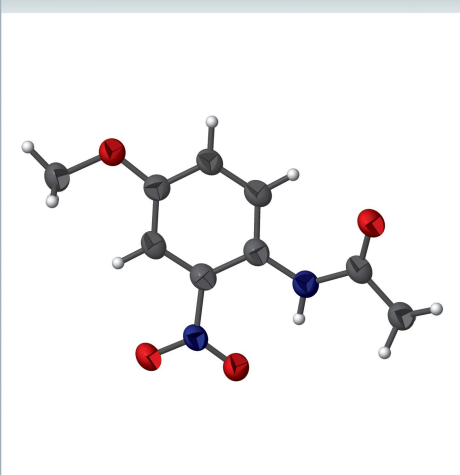
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Keywords: crystal structure; hydrogen bonding.

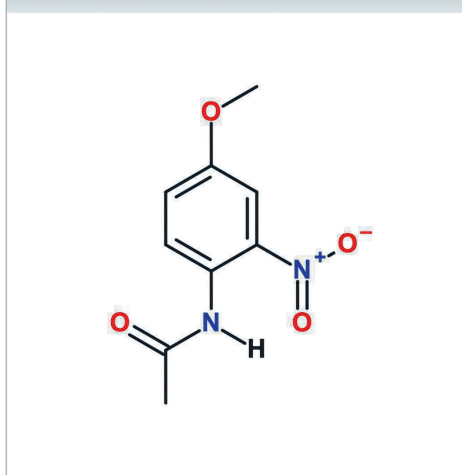
Structural data: full structural data are available from [iucrdata.iucr.org](http://iucrdata.iucr.org)

In the title compound, C<sub>9</sub>H<sub>10</sub>N<sub>2</sub>O<sub>4</sub>, the three substituents vary in the degree of lack of planarity with the central phenyl ring. The methoxy group is nearest to being coplanar, with a C—C—O—C torsion angle of 6.1 (5)°. The nitro group is less coplanar, with a 12.8 (5)° twist about the C—N bond and the acetamido group is considerably less coplanar with the central ring, having a 25.4 (5)° twist about the C—N bond to the ring. The NH group forms an intramolecular N—H···O hydrogen bond to a nitro-group O atom.

## 3D view

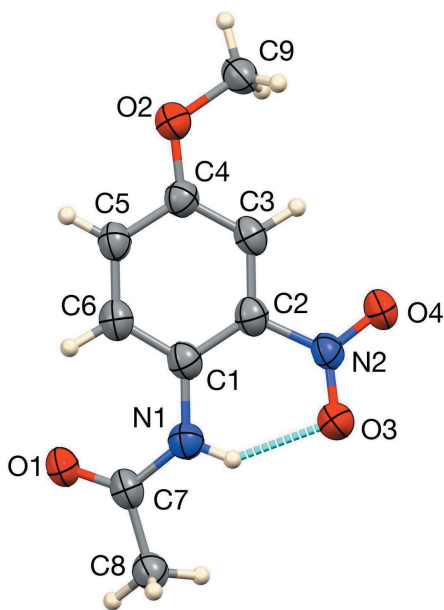


## Chemical scheme



## Structure description

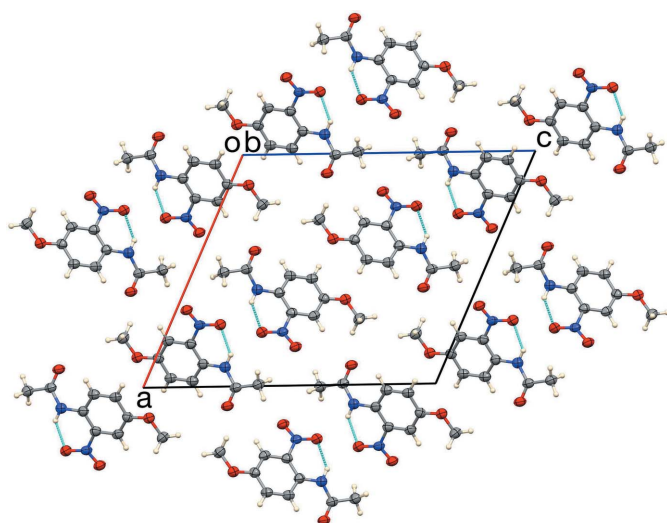
The analgesic use of 4-alkoxyacetanilides, in particular 4-ethoxyacetanilide or 4-EA, predates the First World War. 4-Hydroxyacetanilide (popularly known as Tylenol or acetaminophen) and 4-EA were introduced into the markets at around the same time; however, 4-EA was withdrawn from sale some decades ago due to its carcinogenic and kidney-damaging properties (Dubach *et al.*, 1983; Nakanishi *et al.*, 1982). Although there has been extensive information on phase I and phase II biotransformation of 4-alkoxyacetanilides (Hinson, 1983; Kapetanović *et al.*, 1979; Mulder *et al.*, 1984; Veronese *et al.*, 1985), little or no information is available on nitrated or other oxidation products that could be formed in reactions with cellular oxidants, such as hypochlorite (<sup>-</sup>OCl)/hypochlorous acid (HOCl; p*K*<sub>a</sub> ≈ 7.53) and peroxyxynitrite (ONOO<sup>-</sup>)/peroxyxynitrous acid (ONOOH; p*K*<sub>a</sub> ≈ 6.2; ONOOH and ONOO<sup>-</sup> are collectively referred to as peroxyxynitrite or PN). We have shown, for instance, that 4-hydroxyacetanilide forms nitrated and chlorinated products along with varying amounts of dimers when reacted with HOCl/<sup>-</sup>OCl and PN/CO<sub>2</sub> under physiologically relevant conditions (Uppu & Martin, 2005; Deere *et al.*, 2022). We suspect that similar products (or their positional isomers) may be formed in the reactions of 4-alkoxyacetanilides with the cellular oxidants refer-



**Figure 1**  
The title molecule with 50% displacement ellipsoids with the intramolecular N—H···O hydrogen bond shown as a blue dashed line.

enced above. Towards a better understanding of this and to shed light on molecular targets (Bertolini *et al.*, 2006), we have synthesized the title compound,  $C_9H_{10}N_2O_4$ : single crystals grown from aqueous solution were analyzed by X-ray diffraction.

The title compound is shown in Fig. 1. It is significantly non-planar, and its deviation from planarity may be described by torsion angles about bonds from the central C1–C6 phenyl ring to the three substituents. The methoxy group is nearest to being coplanar, with a C9–O2–C4–C3 torsion angle of  $6.1(5)^\circ$ . The nitro group deviates more from coplanarity with the central ring, with the O3–N2–C2–C1 torsion angle



**Figure 2**  
The unit cell, viewed down the [010] direction, showing intramolecular hydrogen bonds.

**Table 1**  
Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1–H1N···O3	0.87 (5)	1.92 (5)	2.632 (4)	137 (4)
C5–H5···O2 <sup>i</sup>	0.95	2.48	3.418 (4)	171
C6–H6···O1	0.95	2.30	2.864 (4)	117
C8–H8B···O3 <sup>ii</sup>	0.98	2.64	3.578 (4)	160
C8–H8C···O4 <sup>iii</sup>	0.98	2.63	3.546 (4)	156

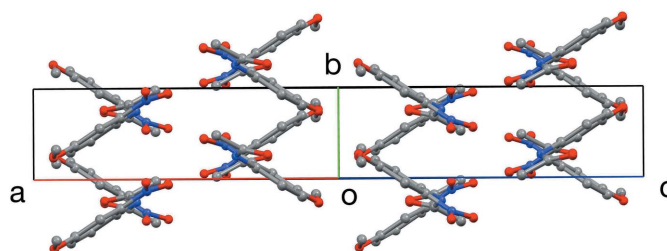
Symmetry codes: (i)  $-x + 1, -y, -z + 1$ ; (ii)  $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{3}{2}$ ; (iii)  $x + \frac{1}{2}, -y + \frac{5}{2}, z + \frac{1}{2}$ .

being  $-12.8(5)^\circ$ . The acetamido group is considerably less coplanar with the central ring, with a C7–N1–C1–C6 torsion angle of  $25.4(5)^\circ$ . These deviations are similar to those seen in the analogous 4-ethoxy compound (Uppu *et al.*, 2020), in which the corresponding torsion angles are  $0.56(12)$ ,  $-14.94(13)$  and  $18.23(15)^\circ$ , respectively. *N*-(4-Hydroxy-2-nitrophenyl)acetamide (Hines *et al.*, 2022) is considerably more planar, with torsion angles to the nitro group and to the acetamido group being  $-0.79(19)$  and  $3.1(2)^\circ$ , respectively, likely as a result of intermolecular hydrogen bonding by the OH group. The structure of *N*-(4-hydroxy-3-nitrophenyl)acetamide, in which the OH group likewise participates in intermolecular hydrogen bonding, has also been reported (Salahifar *et al.*, 2015; Deere *et al.*, 2019). It is also more planar than the title compound, with a torsion angle of  $-11.8(2)^\circ$  for the nitro group and  $9.0(2)^\circ$  for the acetamido group. An intramolecular N1–H1N···O3 hydrogen bond (Table 1) is observed in the title compound.

The unit cell of the title compound is shown in Figs. 2 and 3. The closest intermolecular contact is C5–H5···O2 (at  $1 - x, -y, 1 - z$ ), forming dimers about inversion centers with a  $C\cdots O$  distance of  $3.418(4) \text{ \AA}$  and  $171^\circ$  angle about H. Molecules form a herringbone pattern in the [101] direction with alternate phenyl rings forming a dihedral angle of  $65.7(2)^\circ$ .

### Synthesis and crystallization

*N*-(4-Methoxy-2-nitrophenyl)acetamide was synthesized by acetylation of 4-methoxy-2-nitroaniline using acetic anhydride in acetic acid solvent: 3.36 g (20 mmol) of 4-methoxy-2-nitroaniline in 30 ml of glacial acetic was allowed to react with 2.46 g (24 mmol) of acetic anhydride for 18 h at room temperature. The reaction mixture was stirred continuously during the reaction. In the end, the mixture was dried under



**Figure 3**  
The unit cell, viewed down the [101] direction. H atoms are not shown.

**Table 2**  
Experimental details.

Crystal data	
Chemical formula	C <sub>9</sub> H <sub>10</sub> N <sub>2</sub> O <sub>4</sub>
<i>M<sub>r</sub></i>	210.19
Crystal system, space group	Monoclinic, <i>P</i> 2 <sub>1</sub> / <i>n</i>
Temperature (K)	90
<i>a</i> , <i>b</i> , <i>c</i> (Å)	14.8713 (7), 3.9563 (2), 17.2057 (9)
$\beta$ (°)	114.051 (3)
<i>V</i> (Å <sup>3</sup> )	924.42 (8)
<i>Z</i>	4
Radiation type	Cu <i>K</i> $\alpha$
$\mu$ (mm <sup>-1</sup> )	1.03
Crystal size (mm)	0.42 × 0.06 × 0.01
Data collection	
Diffractionmeter	Bruker Kappa APEXII DUO CCD
Absorption correction	Multi-scan ( <i>SADABS</i> ; Krause <i>et al.</i> , 2015)
<i>T</i> <sub>min</sub> , <i>T</i> <sub>max</sub>	0.692, 0.990
No. of measured, independent and observed [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )] reflections	11516, 1638, 1211
<i>R</i> <sub>int</sub>	0.122
( $\sin \theta/\lambda$ ) <sub>max</sub> (Å <sup>-1</sup> )	0.595
Refinement	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2 $\sigma$ ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.071, 0.203, 1.09
No. of reflections	1638
No. of parameters	141
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\text{max}}$ , $\Delta\rho_{\text{min}}$ (e Å <sup>-3</sup> )	0.24, -0.27

Computer programs: *APEX2* and *SAINTE* (Bruker, 2016), *SHELXT2014/5* (Sheldrick, 2008), *SHELXL2017/1* (Sheldrick, 2015), *Mercury* (Macrae *et al.*, 2020), and *publCIF* (Westrip, 2010).

vacuum, and the *N*-(4-methoxy-2-nitrophenyl)acetamide in the residue was purified by recrystallization twice from aqueous solution. Single crystals in the form of yellow laths were grown in water by slow cooling of a hot and nearly saturated solution of the title compound.

## Refinement

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

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## full crystallographic data

*IUCrData* (2022). 7, x220277 [https://doi.org/10.1107/S2414314622002772]

*N*-(4-Methoxy-2-nitrophenyl)acetamide

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*N*-(4-Methoxy-2-nitrophenyl)acetamide*Crystal data*

$C_9H_{10}N_2O_4$

$M_r = 210.19$

Monoclinic,  $P2_1/n$

$a = 14.8713$  (7) Å

$b = 3.9563$  (2) Å

$c = 17.2057$  (9) Å

$\beta = 114.051$  (3)°

$V = 924.42$  (8) Å<sup>3</sup>

$Z = 4$

$F(000) = 440$

$D_x = 1.510$  Mg m<sup>-3</sup>

Cu  $K\alpha$  radiation,  $\lambda = 1.54184$  Å

Cell parameters from 2102 reflections

$\theta = 3.3$ – $66.3$ °

$\mu = 1.03$  mm<sup>-1</sup>

$T = 90$  K

Lath, yellow

$0.42 \times 0.06 \times 0.01$  mm

*Data collection*

Bruker Kappa APEXII DUO CCD  
diffractometer

Radiation source:  $I\mu$ S microfocus

QUAZAR multilayer optics monochromator

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan  
(SADABS; Krause *et al.*, 2015)

$T_{\min} = 0.692$ ,  $T_{\max} = 0.990$

11516 measured reflections

1638 independent reflections

1211 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.122$

$\theta_{\max} = 66.7$ °,  $\theta_{\min} = 3.3$ °

$h = -17 \rightarrow 17$

$k = -4 \rightarrow 4$

$l = -20 \rightarrow 20$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.071$

$wR(F^2) = 0.203$

$S = 1.09$

1638 reflections

141 parameters

0 restraints

Hydrogen site location: mixed

H atoms treated by a mixture of independent  
and constrained refinement

$w = 1/[\sigma^2(F_o^2) + 0.298P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.24$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.27$  e Å<sup>-3</sup>

*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.** All H atoms were located in difference maps and those on C were thereafter treated as riding in geometrically idealized positions with C—H distances 0.95 Å for phenyl and 0.98 Å for methyl. Coordinates of the N—H hydrogen atom were refined.  $U_{\text{iso}}(\text{H})$  values were assigned as  $1.2U_{\text{eq}}$  for the attached atom (1.5 for methyl).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.58485 (18)	0.7604 (7)	0.81731 (16)	0.0512 (7)
O2	0.36866 (18)	0.2368 (6)	0.43490 (15)	0.0455 (6)
O3	0.23210 (18)	0.9412 (7)	0.67288 (16)	0.0529 (7)
O4	0.16683 (18)	0.9595 (6)	0.53559 (16)	0.0480 (7)
N1	0.4165 (2)	0.7462 (7)	0.75182 (18)	0.0447 (7)
H1N	0.363 (4)	0.830 (11)	0.753 (3)	0.054*
N2	0.2326 (2)	0.8718 (7)	0.60286 (18)	0.0416 (7)
C1	0.4018 (3)	0.6185 (9)	0.6716 (2)	0.0428 (8)
C2	0.3144 (2)	0.6751 (8)	0.5992 (2)	0.0420 (8)
C3	0.3005 (2)	0.5555 (8)	0.5182 (2)	0.0415 (8)
H3A	0.241073	0.602472	0.470197	0.050*
C4	0.3736 (3)	0.3699 (8)	0.5092 (2)	0.0417 (8)
C5	0.4605 (3)	0.3057 (8)	0.5806 (2)	0.0431 (8)
H5	0.511084	0.176401	0.574482	0.052*
C6	0.4740 (3)	0.4264 (9)	0.6593 (2)	0.0442 (8)
H6	0.533915	0.378381	0.706654	0.053*
C7	0.5054 (3)	0.8178 (8)	0.8187 (2)	0.0435 (8)
C8	0.4928 (3)	0.9743 (9)	0.8926 (2)	0.0475 (8)
H8A	0.473964	0.799894	0.923540	0.071*
H8B	0.441299	1.147414	0.872021	0.071*
H8C	0.554993	1.078496	0.930706	0.071*
C9	0.2843 (3)	0.3245 (9)	0.3589 (2)	0.0488 (9)
H9A	0.224837	0.228708	0.361637	0.073*
H9B	0.292327	0.233462	0.309172	0.073*
H9C	0.278101	0.571021	0.354165	0.073*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0331 (14)	0.0634 (15)	0.0497 (14)	0.0015 (10)	0.0093 (11)	-0.0066 (11)
O2	0.0413 (14)	0.0494 (13)	0.0439 (13)	-0.0005 (10)	0.0154 (10)	-0.0013 (10)
O3	0.0419 (14)	0.0706 (16)	0.0434 (14)	0.0026 (12)	0.0145 (11)	-0.0053 (11)
O4	0.0361 (13)	0.0553 (14)	0.0444 (13)	0.0047 (10)	0.0079 (10)	0.0026 (10)
N1	0.0398 (17)	0.0513 (16)	0.0424 (15)	0.0000 (12)	0.0162 (13)	0.0006 (12)
N2	0.0308 (15)	0.0463 (15)	0.0425 (16)	-0.0030 (11)	0.0097 (13)	-0.0028 (12)
C1	0.0376 (18)	0.0453 (17)	0.0429 (18)	-0.0019 (13)	0.0140 (15)	0.0030 (13)
C2	0.0354 (18)	0.0430 (17)	0.0458 (19)	-0.0024 (13)	0.0148 (15)	0.0032 (13)
C3	0.0342 (17)	0.0411 (17)	0.0432 (17)	-0.0037 (13)	0.0095 (14)	0.0033 (13)
C4	0.0381 (18)	0.0425 (17)	0.0446 (18)	-0.0025 (13)	0.0170 (15)	-0.0011 (13)
C5	0.0331 (18)	0.0454 (17)	0.0469 (19)	-0.0008 (13)	0.0125 (15)	-0.0009 (14)
C6	0.0366 (18)	0.0437 (17)	0.0495 (19)	0.0007 (13)	0.0146 (15)	0.0033 (14)
C7	0.0342 (19)	0.0449 (17)	0.0452 (18)	-0.0005 (13)	0.0099 (15)	0.0039 (13)
C8	0.0412 (19)	0.0501 (19)	0.0462 (18)	0.0005 (15)	0.0126 (15)	-0.0017 (15)
C9	0.045 (2)	0.0517 (19)	0.0416 (18)	0.0030 (15)	0.0089 (16)	-0.0008 (14)

*Geometric parameters (Å, °)*

O1—C7	1.214 (4)	C3—H3A	0.9500
O2—C4	1.357 (4)	C4—C5	1.395 (5)
O2—C9	1.438 (4)	C5—C6	1.371 (5)
O3—N2	1.239 (4)	C5—H5	0.9500
O4—N2	1.222 (4)	C6—H6	0.9500
N1—C7	1.383 (5)	C7—C8	1.492 (5)
N1—C1	1.401 (5)	C8—H8A	0.9800
N1—H1N	0.87 (5)	C8—H8B	0.9800
N2—C2	1.467 (4)	C8—H8C	0.9800
C1—C6	1.400 (5)	C9—H9A	0.9800
C1—C2	1.405 (5)	C9—H9B	0.9800
C2—C3	1.404 (5)	C9—H9C	0.9800
C3—C4	1.372 (5)		
C4—O2—C9	117.1 (3)	C6—C5—H5	119.5
C7—N1—C1	127.4 (3)	C4—C5—H5	119.5
C7—N1—H1N	118 (3)	C5—C6—C1	121.7 (3)
C1—N1—H1N	113 (3)	C5—C6—H6	119.1
O4—N2—O3	122.6 (3)	C1—C6—H6	119.1
O4—N2—C2	117.9 (3)	O1—C7—N1	123.6 (3)
O3—N2—C2	119.6 (3)	O1—C7—C8	123.8 (3)
C6—C1—N1	121.6 (3)	N1—C7—C8	112.7 (3)
C6—C1—C2	116.2 (3)	C7—C8—H8A	109.5
N1—C1—C2	122.2 (3)	C7—C8—H8B	109.5
C3—C2—C1	122.4 (3)	H8A—C8—H8B	109.5
C3—C2—N2	115.6 (3)	C7—C8—H8C	109.5
C1—C2—N2	122.0 (3)	H8A—C8—H8C	109.5
C4—C3—C2	119.2 (3)	H8B—C8—H8C	109.5
C4—C3—H3A	120.4	O2—C9—H9A	109.5
C2—C3—H3A	120.4	O2—C9—H9B	109.5
O2—C4—C3	124.9 (3)	H9A—C9—H9B	109.5
O2—C4—C5	115.7 (3)	O2—C9—H9C	109.5
C3—C4—C5	119.4 (3)	H9A—C9—H9C	109.5
C6—C5—C4	121.0 (3)	H9B—C9—H9C	109.5
C7—N1—C1—C6	25.4 (5)	C9—O2—C4—C3	6.1 (5)
C7—N1—C1—C2	-154.6 (3)	C9—O2—C4—C5	-174.3 (3)
C6—C1—C2—C3	-1.8 (5)	C2—C3—C4—O2	179.1 (3)
N1—C1—C2—C3	178.2 (3)	C2—C3—C4—C5	-0.4 (5)
C6—C1—C2—N2	180.0 (3)	O2—C4—C5—C6	-179.9 (3)
N1—C1—C2—N2	-0.1 (5)	C3—C4—C5—C6	-0.3 (5)
O4—N2—C2—C3	-10.9 (4)	C4—C5—C6—C1	-0.1 (5)
O3—N2—C2—C3	168.8 (3)	N1—C1—C6—C5	-178.9 (3)
O4—N2—C2—C1	167.5 (3)	C2—C1—C6—C5	1.1 (5)
O3—N2—C2—C1	-12.8 (5)	C1—N1—C7—O1	-3.9 (6)
C1—C2—C3—C4	1.5 (5)	C1—N1—C7—C8	175.8 (3)

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N2—C2—C3—C4                      179.9 (3)

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*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
N1—H1N $\cdots$ O3	0.87 (5)	1.92 (5)	2.632 (4)	137 (4)
C5—H5 $\cdots$ O2 <sup>i</sup>	0.95	2.48	3.418 (4)	171
C6—H6 $\cdots$ O1	0.95	2.30	2.864 (4)	117
C8—H8B $\cdots$ O3 <sup>ii</sup>	0.98	2.64	3.578 (4)	160
C8—H8C $\cdots$ O4 <sup>iii</sup>	0.98	2.63	3.546 (4)	156

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Symmetry codes: (i)  $-x+1, -y, -z+1$ ; (ii)  $-x+1/2, y+1/2, -z+3/2$ ; (iii)  $x+1/2, -y+5/2, z+1/2$ .