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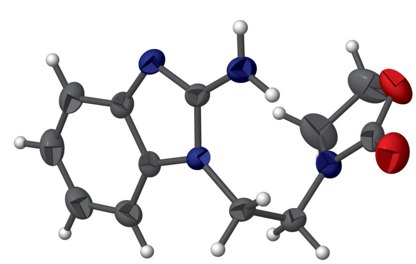
3-[2-(2-Amino-1*H*-benzo[*d*]imidazol-1-yl)ethyl]-1,3-oxazolidin-2-one

Abdellatif Bouayyadi,[a,b]* Ahmed Moussaif,[b] Abdelhalim Mesfioui,[a] Mohammed Mzibri,[b] Mohamed Saadi[c] and Lahcen El Ammari[c]

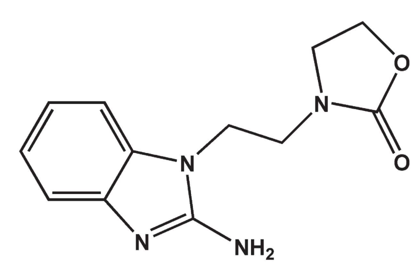
[a]Laboratory of Genetic, Endocrinology and Biotechnology–Faculty of Sciences, Ibn Tofaïl University, Kenitra, Morocco, [b]National Center of Energy Sciences and Nuclear Techniques, Rabat, Morocco, and [c]Laboratoire de Chimie du Solide Appliquée, Faculty of Sciences, Mohammed V University in Rabat, Avenue Ibn Battouta, BP 1014, Rabat, Morocco. *Correspondence e-mail: abouayyadi@yahoo.com

In the title compound, $C_{12}H_{14}N_4O_2$, the benzimidazole ring is almost planar (r.m.s. deviation = 0.03 Å), with the fused ring system slightly folded at the shared atoms, with a dihedral angle of 3.4 (1)°. The oxazolidinone ring displays a twisted conformation on the $-CH_2-CH_2-$ bond and its mean plane makes a dihedral angle of 57.4 (1)° with the benzimidazole ring mean plane. In the crystal, molecules are linked by N—H···O and N—H···N hydrogen bonds, forming chains propagating along the *a*-axis direction. The chains are linked by C—H···O and C—H···N hydrogen bonds, forming a three-dimensional structure, which is reinforced by C—H···π interactions.

3D view



Chemical scheme



Structure description

Molecules containing an heterocycle, include compounds with organic, chemical and many pharmacological interests (Komeilizadeh, 2006). Two-thirds of organic compounds, known in the literature, are heterocyclic (Brandi *et al.*, 2003; Ansar *et al.*, 2009). Benzimidazole and oxazoline derivatives have attracted considerable interest because of their important biological activities, such as antidepressant and anxiolytic (Ahabchane *et al.*, 1999, 2000; Alinezhad *et al.*, 2013; Ansari & Lal, 2009). The importance of these pharmacological activities encouraged us to combine both benzimidazole and oxazoline units in one molecule and to assess their toxicity (acute and chronic), and also their psychotropic activity. It involves the synthesis by the transfer phase catalysis (PTC) of a novel benzimidazole derivative from 2-amino-benzimidazole, combined with an oxazolidin-2-one unit.

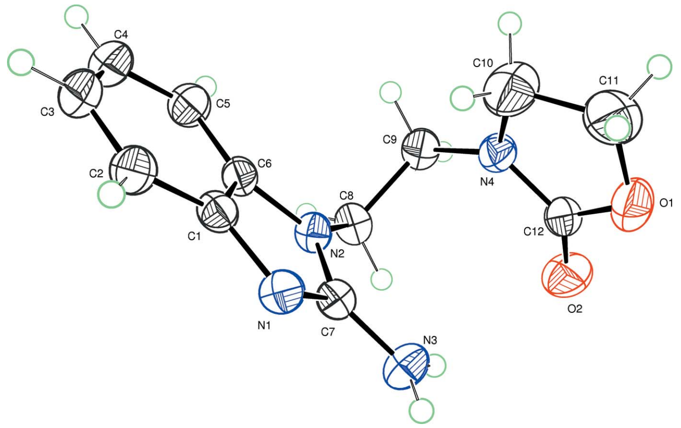


Figure 1
The molecular structure of the title compound, showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

The title compound, Fig. 1, is build up from an amino-benzimidazole ring linked to an oxazolidin-2-on through an ethylene group. The benzimidazole ring is virtually planar with the maximum deviation from the mean plane being 0.037 (2) Å for atom C7. The oxazoline ring displays a twisted conformation on the C10–C11 bond [puckering amplitude $Q2$ = 0.107 (3) Å, and the spherical polar angle $\varphi2$ = 50.5 (2)°]. The dihedral angle between the mean planes of the benzimidazole system and the oxazoline ring is 57.4 (1)°.

In the crystal, molecules are linked by N—H···O and N—H···N hydrogen bonds, forming chains propagating along the *a*-axis direction (Fig. 2 and Table 1). The chains are linked by C—H···O and C—H···N hydrogen bonds, forming a three-dimensional structure, which is reinforced by C—H···π interactions (Fig. 2 and Table 1).

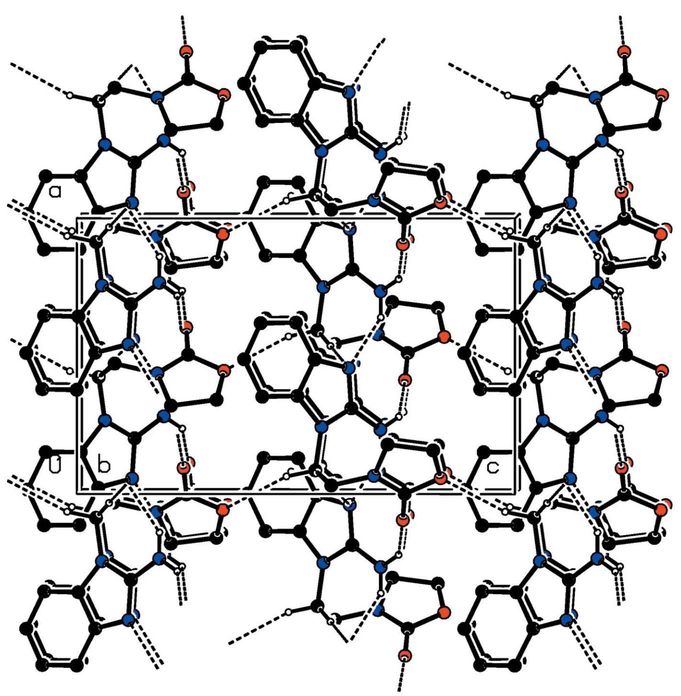


Figure 2
A view along the *b* axis of the crystal packing of the title compound. Hydrogen bonds are shown as dashed lines (see Table 1) and, for clarity, only the H atoms involved in hydrogen bonding have been included.

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

*Cg*1 is the centroid of C1–C6 ring.

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3*A*···O2^{i}	0.86	2.29	2.994 (2)	140
N3—H3*B*···N1^{ii}	0.86	2.39	3.020 (2)	131
C8—H8*A*···O1^{iii}	0.97	2.49	3.410 (3)	158
C8—H8*B*···N1^{ii}	0.97	2.50	3.425 (2)	159
C9—H9*A*···*Cg*1^{iv}	0.97	2.80	3.571 (2)	137
C11—H11*B*···*Cg*1^{v}	0.97	2.80	3.730 (3)	161

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{12}H_{14}N_4O_2$
M_r	246.27
Crystal system, space group	Orthorhombic, $Pna2_1$
Temperature (K)	296
a, b, c (Å)	9.0504 (2), 9.0612 (1), 14.3565 (2)
V (Å^3)	1177.34 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.10
Crystal size (mm)	0.44 × 0.34 × 0.26
Data collection	
Diffractometer	Bruker X8 *APEX*
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.663, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	46121, 3320, 3097
R_{int}	0.034
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.035, 0.100, 1.07
No. of reflections	3320
No. of parameters	163
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.20, −0.24
Absolute structure	Flack x determined using 1380 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	−0.3 (3)

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3* Farrugia, 2012), *PLATON* (Spek, 2009), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

Synthesis and crystallization

Phase transfer catalysis (PTC) is a well established technique, widely used in synthetic chemistry and applied in many industrial processes. Here, we present the principle of the PTC and its benefits for the development of more eco-friendly processes. The alkylation reaction, from the starting product of 2-amino-benzimidazole, was carried out under the same reaction conditions, to form an oxazolidin-2-one unit, which was alkylated to the benzimidazole unit.

To the solution of 2-amino-benzimidazole (1.35 g, 9 mmol) and dichloroethyl amine hydrochloride (2.41 g, 13.5 mmol) in dimethylformamide (80 ml) were added potassium carbonate (4.14 g, 30 mmol) and tetra-*n*-butylammonium bromide (0.10 g, 0.3 mmol). The resulting mixture was refluxed for 4 h, then filtered and the solvent removed. The residue was purified by column chromatography on silica gel (hexane/AcOEt: 60/40) to afford the title compound (Yield 70%, m.p. 504 K). ^{1}H NMR (dppm): 3.35: SCH_2 (2H, *t*, J = 6.3 Hz); 3.37: NCH_2 (4H, *m*); 4.16: OCH_2 (2H, *t*, J = 6.6 Hz); 7.09–7.12: CH-benzenic (4H, *m*); 12.54: NH (1H, *s*).

Refinement

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

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x161895 [https://doi.org/10.1107/S2414314616018952]

3-[2-(2-Amino-1*H*-benzo[*d*]imidazol-1-yl)ethyl]-1,3-oxazolidin-2-one

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Crystal data

$C_{12}H_{14}N_4O_2$
$M_r = 246.27$
Orthorhombic, $Pna2_1$
$a = 9.0504$ (2) Å
$b = 9.0612$ (1) Å
$c = 14.3565$ (2) Å
$V = 1177.34$ (3) Å^3
$Z = 4$
$F(000) = 520$
$D_x = 1.389$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3320 reflections
$\theta = 2.7$–29.6°
$\mu = 0.10$ mm^{-1}
$T = 296$ K
Block, colourless
0.44 × 0.34 × 0.26 mm

Data collection

Bruker X8 APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
$T_{min} = 0.663$, $T_{max} = 0.746$
46121 measured reflections
3320 independent reflections
3097 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 29.6°$, $\theta_{min} = 2.7°$
$h = -12 \rightarrow 12$
$k = -12 \rightarrow 12$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.100$
$S = 1.07$
3320 reflections
163 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0582P)^2 + 0.1462P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.20$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}
Absolute structure: Flack x determined using 1380 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013)
Absolute structure parameter: −0.3 (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.

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

	x	y	z	U_{iso}*/U_{eq}
C1	0.98692 (19)	0.55021 (18)	0.54222 (14)	0.0305 (3)
C2	1.1216 (2)	0.5197 (2)	0.49961 (18)	0.0408 (4)
H2	1.2096	0.5567	0.5237	0.049*
C3	1.1210 (3)	0.4324 (2)	0.42002 (19)	0.0480 (5)
H3	1.2102	0.4110	0.3908	0.058*
C4	0.9909 (3)	0.3764 (2)	0.38293 (17)	0.0479 (5)
H4	0.9947	0.3177	0.3298	0.057*
C5	0.8550 (2)	0.4067 (2)	0.42404 (15)	0.0396 (4)
H5	0.7674	0.3698	0.3995	0.047*
C6	0.85612 (19)	0.49410 (19)	0.50313 (13)	0.0292 (3)
C7	0.80874 (18)	0.63783 (18)	0.62457 (12)	0.0276 (3)
C8	0.58530 (19)	0.5271 (2)	0.54381 (13)	0.0318 (4)
H8A	0.5635	0.5317	0.4777	0.038*
H8B	0.5305	0.6055	0.5743	0.038*
C9	0.5335 (2)	0.3792 (2)	0.58184 (13)	0.0346 (4)
H9A	0.4274	0.3718	0.5737	0.042*
H9B	0.5788	0.3009	0.5457	0.042*
C10	0.6839 (4)	0.2609 (4)	0.7117 (2)	0.0633 (8)
H10A	0.7806	0.2972	0.6936	0.076*
H10B	0.6712	0.1612	0.6884	0.076*
C11	0.6626 (4)	0.2679 (3)	0.8156 (2)	0.0661 (8)
H11A	0.6234	0.1753	0.8389	0.079*
H11B	0.7557	0.2879	0.8466	0.079*
C12	0.5022 (2)	0.4301 (2)	0.74885 (15)	0.0357 (4)
N1	0.95466 (16)	0.63860 (17)	0.61871 (12)	0.0322 (3)
N2	0.74285 (16)	0.55200 (16)	0.55759 (10)	0.0285 (3)
N3	0.73039 (18)	0.71167 (19)	0.69026 (12)	0.0362 (3)
H3A	0.7756	0.7632	0.7317	0.043*
H3B	0.6355	0.7069	0.6905	0.043*
N4	0.56840 (19)	0.35663 (18)	0.67963 (12)	0.0337 (3)
O1	0.5596 (3)	0.3860 (2)	0.83151 (12)	0.0560 (5)
O2	0.4053 (2)	0.52092 (19)	0.74365 (15)	0.0548 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0284 (8)	0.0282 (7)	0.0350 (9)	−0.0007 (6)	0.0017 (7)	0.0036 (7)
C2	0.0310 (8)	0.0388 (9)	0.0526 (12)	0.0001 (7)	0.0087 (9)	0.0003 (9)
C3	0.0476 (12)	0.0429 (10)	0.0534 (13)	0.0076 (9)	0.0210 (10)	0.0027 (10)

C4	0.0621 (14)	0.0433 (10)	0.0383 (11)	0.0036 (10)	0.0122 (10)	−0.0042 (9)
C5	0.0464 (11)	0.0388 (9)	0.0335 (9)	−0.0026 (8)	0.0000 (8)	−0.0018 (8)
C6	0.0301 (7)	0.0289 (7)	0.0286 (8)	−0.0002 (6)	0.0030 (7)	0.0041 (6)
C7	0.0263 (7)	0.0289 (7)	0.0276 (7)	−0.0008 (6)	−0.0032 (6)	0.0024 (6)
C8	0.0257 (7)	0.0387 (8)	0.0312 (9)	−0.0022 (6)	−0.0056 (7)	0.0034 (7)
C9	0.0317 (8)	0.0397 (9)	0.0325 (9)	−0.0070 (7)	−0.0013 (7)	−0.0038 (7)
C10	0.0683 (17)	0.0687 (17)	0.0529 (13)	0.0356 (14)	−0.0008 (13)	0.0052 (12)
C11	0.093 (2)	0.0564 (15)	0.0491 (14)	0.0210 (15)	−0.0150 (15)	0.0098 (12)
C12	0.0363 (9)	0.0335 (8)	0.0373 (9)	−0.0036 (7)	0.0085 (8)	−0.0001 (8)
N1	0.0249 (6)	0.0339 (7)	0.0377 (8)	−0.0011 (6)	−0.0009 (6)	−0.0027 (6)
N2	0.0240 (6)	0.0331 (7)	0.0282 (7)	−0.0026 (5)	−0.0008 (5)	−0.0002 (5)
N3	0.0268 (7)	0.0458 (8)	0.0362 (8)	0.0023 (6)	−0.0011 (6)	−0.0089 (7)
N4	0.0347 (8)	0.0340 (7)	0.0325 (8)	0.0049 (6)	0.0030 (6)	0.0008 (6)
O1	0.0754 (12)	0.0597 (10)	0.0330 (7)	0.0104 (9)	0.0072 (8)	0.0016 (7)
O2	0.0462 (8)	0.0498 (9)	0.0685 (12)	0.0139 (7)	0.0149 (9)	−0.0051 (8)

Geometric parameters (Å, º)

C1—N1	1.390 (3)	C8—H8A	0.9700
C1—C2	1.392 (3)	C8—H8B	0.9700
C1—C6	1.405 (2)	C9—N4	1.453 (3)
C2—C3	1.390 (4)	C9—H9A	0.9700
C2—H2	0.9300	C9—H9B	0.9700
C3—C4	1.388 (4)	C10—N4	1.434 (3)
C3—H3	0.9300	C10—C11	1.506 (4)
C4—C5	1.392 (3)	C10—H10A	0.9700
C4—H4	0.9300	C10—H10B	0.9700
C5—C6	1.384 (3)	C11—O1	1.437 (3)
C5—H5	0.9300	C11—H11A	0.9700
C6—N2	1.392 (2)	C11—H11B	0.9700
C7—N1	1.323 (2)	C12—O2	1.206 (3)
C7—N3	1.356 (2)	C12—N4	1.337 (3)
C7—N2	1.373 (2)	C12—O1	1.356 (3)
C8—N2	1.457 (2)	N3—H3A	0.8600
C8—C9	1.522 (3)	N3—H3B	0.8600
N1—C1—C2	130.21 (18)	N4—C9—H9B	108.8
N1—C1—C6	110.30 (15)	C8—C9—H9B	108.8
C2—C1—C6	119.38 (18)	H9A—C9—H9B	107.7
C3—C2—C1	118.1 (2)	N4—C10—C11	101.5 (2)
C3—C2—H2	121.0	N4—C10—H10A	111.5
C1—C2—H2	121.0	C11—C10—H10A	111.5
C4—C3—C2	121.8 (2)	N4—C10—H10B	111.5
C4—C3—H3	119.1	C11—C10—H10B	111.5
C2—C3—H3	119.1	H10A—C10—H10B	109.3
C3—C4—C5	121.0 (2)	O1—C11—C10	105.8 (2)
C3—C4—H4	119.5	O1—C11—H11A	110.6
C5—C4—H4	119.5	C10—C11—H11A	110.6

C6—C5—C4	117.0 (2)	O1—C11—H11B	110.6
C6—C5—H5	121.5	C10—C11—H11B	110.6
C4—C5—H5	121.5	H11A—C11—H11B	108.7
C5—C6—N2	132.14 (17)	O2—C12—N4	128.3 (2)
C5—C6—C1	122.73 (17)	O2—C12—O1	122.3 (2)
N2—C6—C1	105.05 (16)	N4—C12—O1	109.41 (17)
N1—C7—N3	124.29 (17)	C7—N1—C1	104.88 (15)
N1—C7—N2	113.07 (16)	C7—N2—C6	106.68 (14)
N3—C7—N2	122.63 (15)	C7—N2—C8	127.43 (15)
N2—C8—C9	112.90 (15)	C6—N2—C8	125.88 (15)
N2—C8—H8A	109.0	C7—N3—H3A	120.0
C9—C8—H8A	109.0	C7—N3—H3B	120.0
N2—C8—H8B	109.0	H3A—N3—H3B	120.0
C9—C8—H8B	109.0	C12—N4—C10	112.89 (19)
H8A—C8—H8B	107.8	C12—N4—C9	123.40 (17)
N4—C9—C8	113.80 (16)	C10—N4—C9	123.59 (19)
N4—C9—H9A	108.8	C12—O1—C11	109.20 (18)
C8—C9—H9A	108.8		

N1—C1—C2—C3	−176.61 (19)	N1—C7—N2—C8	−179.77 (16)
C6—C1—C2—C3	−0.8 (3)	N3—C7—N2—C8	1.1 (3)
C1—C2—C3—C4	0.1 (3)	C5—C6—N2—C7	−176.61 (19)
C2—C3—C4—C5	0.5 (4)	C1—C6—N2—C7	0.17 (18)
C3—C4—C5—C6	−0.2 (3)	C5—C6—N2—C8	2.3 (3)
C4—C5—C6—N2	175.75 (19)	C1—C6—N2—C8	179.11 (16)
C4—C5—C6—C1	−0.6 (3)	C9—C8—N2—C7	−101.4 (2)
N1—C1—C6—C5	177.68 (17)	C9—C8—N2—C6	79.8 (2)
C2—C1—C6—C5	1.1 (3)	O2—C12—N4—C10	177.6 (3)
N1—C1—C6—N2	0.51 (19)	O1—C12—N4—C10	−3.2 (3)
C2—C1—C6—N2	−176.04 (17)	O2—C12—N4—C9	1.5 (3)
N2—C8—C9—N4	55.4 (2)	O1—C12—N4—C9	−179.31 (18)
N4—C10—C11—O1	−10.9 (4)	C11—C10—N4—C12	8.9 (3)
N3—C7—N1—C1	−179.78 (16)	C11—C10—N4—C9	−175.0 (2)
N2—C7—N1—C1	1.1 (2)	C8—C9—N4—C12	70.4 (2)
C2—C1—N1—C7	175.1 (2)	C8—C9—N4—C10	−105.2 (3)
C6—C1—N1—C7	−1.0 (2)	O2—C12—O1—C11	174.7 (2)
N1—C7—N2—C6	−0.9 (2)	N4—C12—O1—C11	−4.5 (3)
N3—C7—N2—C6	−179.95 (16)	C10—C11—O1—C12	9.9 (4)

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of C1–C6 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···O2^{i}	0.86	2.29	2.994 (2)	140
N3—H3*B*···N1^{ii}	0.86	2.39	3.020 (2)	131
C8—H8*A*···O1^{iii}	0.97	2.49	3.410 (3)	158
C8—H8*B*···N1^{ii}	0.97	2.50	3.425 (2)	159

C9—H9*A*···*Cg*1^{iv}	0.97	2.80	3.571 (2)	137
C11—H11*B*···*Cg*1^{v}	0.97	2.80	3.730 (3)	161

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