

Dipentyl 2,6-diaminobenzo[1,2-*b*:4,5-*b'*]-difuran-3,7-dicarboxylate

Giuseppina Roviello,^a Fabio Borbone,^b Antonio Carella,^b Giovanni N. Roviello^{c*} and Angela Tuzi^{b*}

^aDipartimento di Ingegneria, Università di Napoli 'Parthenope', Centro Direzionale di Napoli, Isola C4, 80143 Napoli, Italy, ^bDipartimento di Scienze Chimiche, Università degli Studi di Napoli 'Federico II', Complesso di Monte S. Angelo, Via Cinthia, 80126 Napoli, Italy, and ^cIstituto di Biostrutture e Bioimmagini, CNR, Via Mezzocannone 16, 80134 Naples, Italy

Correspondence e-mail: giuseppina.roviello@uniparthenope.it, angela.tuzi@unina.it

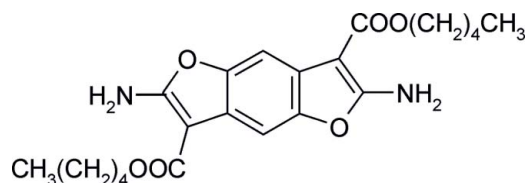
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Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.055; wR factor = 0.134; data-to-parameter ratio = 18.5.

The title compound, $\text{C}_{22}\text{H}_{28}\text{N}_2\text{O}_6$, crystallizes with one half-molecule in the independent unit, the molecule being located on an inversion centre. The pentyl groups are in the all-*trans* conformation and an almost planar conformation of the whole molecule is observed [maximum deviation from the least-squares plane through all non-H atoms is 0.0229 (17) Å for an N atom]. The amino groups are involved in intra- and intermolecular hydrogen bonds. Intramolecular hydrogen bonding involving the amino group and ester carbonyl helps to lock the *syn* conformation of the ester with respect to the amino group. In the crystal, $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonding involving the amino group and the furan and ester carbonyl O atoms self-assembles the molecules into a two-dimensional hydrogen-bonded network parallel to (010) that displays interdigitial packing sustained by alkyl-alkyl interactions.

Related literature

For the synthesis and properties of aminobenzodifurane derivatives, see: Caruso *et al.* (2009). For O- and N-rich aromatic heterocycles, see: Roviello *et al.* (2007, 2012). For molecules with optical and opto-electronical properties, see: Carella *et al.* (2012); Centore *et al.* (2007); Roviello *et al.* (2009); Ricciotti *et al.* (2013); Vitaliano *et al.* (2009). For hydrogen bonding in heterocycles, see: Centore *et al.* (2013a,b).



Experimental

Crystal data

$\text{C}_{22}\text{H}_{28}\text{N}_2\text{O}_6$
 $M_r = 416.46$
 Monoclinic, $P2_1/c$
 $a = 8.267$ (1) Å
 $b = 7.994$ (1) Å
 $c = 17.582$ (3) Å
 $\beta = 98.98$ (2)°

$V = 1147.7$ (3) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.09$ mm⁻¹
 $T = 173$ K
 $0.50 \times 0.04 \times 0.01$ mm

Data collection

Bruker-Nonius KappaCCD diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2001)
 $T_{\min} = 0.957$, $T_{\max} = 0.999$

11093 measured reflections
 2626 independent reflections
 1258 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.096$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.055$
 $wR(F^2) = 0.134$
 $S = 0.93$
 2626 reflections
 142 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.19$ e Å⁻³
 $\Delta\rho_{\min} = -0.20$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1A}\cdots\text{O2}^i$	0.83 (2)	2.11 (2)	2.935 (3)	171 (2)
$\text{N1}-\text{H1B}\cdots\text{O1}^{ii}$	0.84 (2)	2.34 (2)	3.066 (2)	144 (2)
$\text{N1}-\text{H1B}\cdots\text{O2}$	0.84 (2)	2.41 (2)	2.942 (3)	122.2 (18)

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

Data collection: COLLECT (Nonius, 1999); cell refinement: DIRAX/LSQ (Duisenberg *et al.*, 2000); data reduction: EVALCCD (Duisenberg *et al.*, 2003); program(s) used to solve structure: SIR97 (Altomare *et al.*, 1999); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 for Windows (Farrugia, 2012) and Mercury (Macrae *et al.*, 2006); software used to prepare material for publication: WinGX (Farrugia, 2012).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DS2234).

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supplementary materials

Acta Cryst. (2013). E69, o1526–o1527 [doi:10.1107/S160053681302480X]

Dipentyl 2,6-diaminobenzo[1,2-*b*:4,5-*b'*]difuran-3,7-dicarboxylate

Giuseppina Roviello, Fabio Borbone, Antonio Carella, Giovanni N. Roviello and Angela Tuzi

1. Comment

In the field of our studies on the synthesis and properties of aminobenzodifurane derivatives (Caruso *et al.* 2009) we prepared the title compound, C₂₂H₂₈N₂O₆. The presence of an aromatic heterocyclic core in the molecule makes this kind of compound interesting in organic electronics (Carella *et al.* 2012; Centore *et al.* 2007). 2,6-diamino-benzo[1,2-*b*:4,5-*b'*]difuran-3,7-dicarboxylic acid (Fig. 1) crystallizes in *P2₁/c* space group with one half molecule in the independent unit. The molecule is located on a crystallographic inversion center and exhibits an all planar shape (maximum deviation from least square plane of the molecule is -0.0229 (17) for N1). The planarity of the molecule is a consequence of the all-*trans* conformation of penthyl groups and of the torsion angle at C6–O3 bond (C4–C6–O3–C7 = 179.7 (2)°). The planar conformation is also stabilized by intramolecular N—H···O=C hydrogen bonds (Table 1). In fact, the intramolecular hydrogen bonding involving the amino group and ester carbonyl helps to lock the *syn* conformation of ester with respect to amino group. The amino NH₂ group is also involved in intermolecular hydrogen bonds, acting as donor towards benzodifurane oxygen (O1) and ester carbonyl oxygen (O2) acceptors (see Table 1). In the crystal packing (Fig. 2), molecules self-assemble into a two-dimensional hydrogen bonded network that display interdigital packing sustained by alkyl-alkyl interactions.

2. Experimental

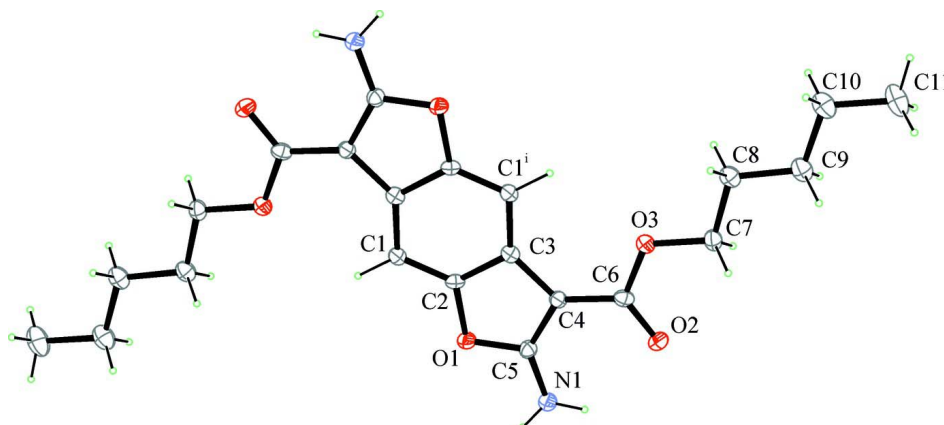
2,6-diamino-benzo[1,2-*b*:4,5-*b'*]difuran-3,7-dicarboxylic acid was prepared according to the procedure described in the literature (Caruso *et al.* 2009). Crystals suitable for X-ray analysis were obtained by slow evaporation of dioxane/water solution.

3. Refinement

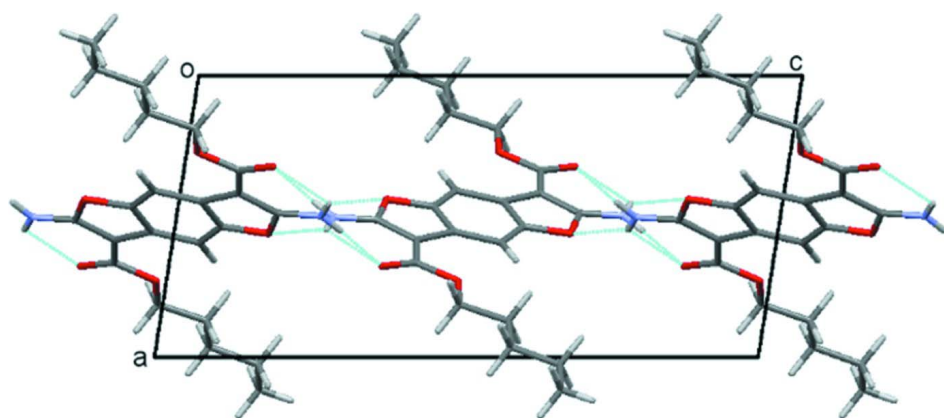
All NH hydrogen atoms were located in difference Fourier maps and refined with $U_{\text{iso}}=1.2U_{\text{eq}}(\text{N})$ of the carrier atom. All the other H atoms were generated stereochemically and refined by the riding model with $U_{\text{iso}}=1.2\times U_{\text{eq}}$ of the carrier atom (1.5 for H atoms of the methyl groups).

Computing details

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *DIRAX/LSQ* (Duisenberg *et al.*, 2000); data reduction: *EVALCCD* (Duisenberg *et al.*, 2003); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

**Figure 1**

ORTEP view of the title compound. Thermal ellipsoids are drawn at 30% probability level.

**Figure 2**

Crystal packing viewed along **b** axis. Hydrogen bonds are drawn as dashed lines.

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Crystal data

$C_{22}H_{28}N_2O_6$

$M_r = 416.46$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2ybc$

$a = 8.267(1)\ \text{\AA}$

$b = 7.994(1)\ \text{\AA}$

$c = 17.582(3)\ \text{\AA}$

$\beta = 98.98(2)^\circ$

$V = 1147.7(3)\ \text{\AA}^3$

$Z = 2$

$F(000) = 444$

$D_x = 1.205\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 75 reflections

$\theta = 3.1\text{--}16.9^\circ$

$\mu = 0.09\ \text{mm}^{-1}$

$T = 173\ \text{K}$

Block, grey

$0.50 \times 0.04 \times 0.01\ \text{mm}$

Data collection

Bruker–Nonius KappaCCD
diffractometer

Radiation source: normal-focus sealed tube

Graphite monochromator

Detector resolution: $9\ \text{pixels mm}^{-1}$

CCD rotation images, thick slices scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2001)

$T_{\min} = 0.957$, $T_{\max} = 0.999$

11093 measured reflections

2626 independent reflections
 1258 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.096$
 $\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 3.2^\circ$

$h = -10 \rightarrow 10$
 $k = -10 \rightarrow 9$
 $l = -22 \rightarrow 22$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.055$
 $wR(F^2) = 0.134$
 $S = 0.93$
 2626 reflections
 142 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 atoms treated by a mixture of independent
 and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.061P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.19 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.20 \text{ e } \text{\AA}^{-3}$

Special details

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.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.5923 (2)	0.1341 (3)	0.04464 (11)	0.0257 (5)
H1	0.6556	0.2314	0.0731	0.026*
C2	0.5354 (2)	-0.0094 (3)	0.07682 (11)	0.0246 (5)
C3	0.4461 (2)	-0.1426 (3)	0.03695 (11)	0.0255 (5)
C4	0.4171 (2)	-0.2648 (3)	0.09645 (11)	0.0254 (5)
C5	0.4884 (3)	-0.1957 (3)	0.16650 (12)	0.0282 (5)
C6	0.3356 (2)	-0.4269 (3)	0.09113 (12)	0.0288 (6)
C7	0.1878 (3)	-0.6355 (3)	0.00858 (11)	0.0326 (6)
H7A	0.0935	-0.6356	0.0370	0.033*
H7B	0.2644	-0.7250	0.0301	0.033*
C8	0.1290 (3)	-0.6679 (3)	-0.07634 (12)	0.0340 (6)
H8A	0.2242	-0.6700	-0.1043	0.034*
H8B	0.0556	-0.5760	-0.0979	0.034*
C9	0.0363 (3)	-0.8366 (3)	-0.08811 (12)	0.0382 (6)
H9A	0.1101	-0.9271	-0.0654	0.038*
H9B	-0.0583	-0.8331	-0.0598	0.038*
C10	-0.0261 (3)	-0.8793 (3)	-0.17302 (13)	0.0472 (7)
H10A	0.0678	-0.8822	-0.2017	0.047*
H10B	-0.1019	-0.7904	-0.1958	0.047*
C11	-0.1155 (4)	-1.0494 (3)	-0.18205 (16)	0.0632 (8)
H11A	-0.1539	-1.0711	-0.2367	0.063*

H11B	-0.2094	-1.0467	-0.1542	0.063*
H11C	-0.0400	-1.1383	-0.1609	0.063*
N1	0.4973 (3)	-0.2479 (3)	0.23935 (11)	0.0383 (6)
H1A	0.550 (3)	-0.192 (3)	0.2748 (12)	0.038*
H1B	0.454 (3)	-0.340 (3)	0.2485 (12)	0.038*
O1	0.56177 (16)	-0.04310 (18)	0.15705 (7)	0.0292 (4)
O2	0.32315 (19)	-0.51874 (18)	0.14725 (8)	0.0377 (4)
O3	0.27143 (17)	-0.47150 (17)	0.01739 (8)	0.0324 (4)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0243 (13)	0.0246 (14)	0.0275 (12)	0.0019 (10)	0.0017 (10)	-0.0028 (10)
C2	0.0267 (12)	0.0283 (14)	0.0184 (11)	0.0051 (11)	0.0018 (9)	0.0001 (10)
C3	0.0225 (12)	0.0268 (14)	0.0271 (12)	0.0040 (10)	0.0039 (10)	-0.0032 (10)
C4	0.0263 (12)	0.0216 (13)	0.0271 (12)	0.0021 (10)	0.0009 (10)	-0.0009 (10)
C5	0.0289 (13)	0.0252 (15)	0.0303 (13)	0.0008 (11)	0.0039 (10)	0.0012 (11)
C6	0.0260 (13)	0.0305 (15)	0.0286 (13)	0.0076 (11)	-0.0001 (10)	-0.0006 (11)
C7	0.0304 (13)	0.0269 (14)	0.0400 (14)	-0.0019 (11)	0.0041 (11)	-0.0014 (11)
C8	0.0282 (13)	0.0345 (16)	0.0385 (13)	0.0024 (11)	0.0029 (11)	-0.0043 (11)
C9	0.0292 (13)	0.0355 (16)	0.0487 (15)	0.0032 (11)	0.0025 (12)	-0.0065 (12)
C10	0.0432 (16)	0.0499 (18)	0.0483 (15)	-0.0056 (14)	0.0068 (13)	-0.0135 (13)
C11	0.0620 (19)	0.054 (2)	0.073 (2)	-0.0181 (16)	0.0085 (16)	-0.0242 (15)
N1	0.0530 (14)	0.0320 (14)	0.0268 (12)	-0.0109 (11)	-0.0033 (10)	0.0022 (10)
O1	0.0350 (9)	0.0296 (10)	0.0224 (8)	-0.0013 (7)	0.0025 (7)	0.0006 (7)
O2	0.0489 (10)	0.0313 (10)	0.0307 (9)	-0.0033 (8)	-0.0003 (7)	0.0075 (7)
O3	0.0373 (9)	0.0293 (10)	0.0289 (9)	-0.0043 (7)	0.0001 (7)	-0.0010 (7)

Geometric parameters (\AA , $^\circ$)

C1—C2	1.393 (3)	C7—H7B	0.9900
C1—C3 ⁱ	1.422 (3)	C8—C9	1.549 (3)
C1—H1	1.0231	C8—H8A	0.9900
C2—C3	1.418 (3)	C8—H8B	0.9900
C2—O1	1.419 (2)	C9—C10	1.540 (3)
C3—C1 ⁱ	1.422 (3)	C9—H9A	0.9900
C3—C4	1.477 (3)	C9—H9B	0.9900
C4—C5	1.394 (3)	C10—C11	1.543 (3)
C4—C6	1.457 (3)	C10—H10A	0.9900
C5—N1	1.338 (3)	C10—H10B	0.9900
C5—O1	1.384 (2)	C11—H11A	0.9800
C6—O2	1.247 (2)	C11—H11B	0.9800
C6—O3	1.369 (2)	C11—H11C	0.9800
C7—O3	1.479 (2)	N1—H1A	0.83 (2)
C7—C8	1.518 (3)	N1—H1B	0.84 (2)
C7—H7A	0.9900		
C2—C1—C3 ⁱ	114.40 (18)	C7—C8—H8B	109.5
C2—C1—H1	127.3	C9—C8—H8B	109.5
C3 ⁱ —C1—H1	118.3	H8A—C8—H8B	108.1

C1—C2—C3	126.93 (18)	C10—C9—C8	114.01 (19)
C1—C2—O1	123.44 (18)	C10—C9—H9A	108.8
C3—C2—O1	109.63 (17)	C8—C9—H9A	108.8
C2—C3—C1 ⁱ	118.67 (18)	C10—C9—H9B	108.8
C2—C3—C4	106.02 (17)	C8—C9—H9B	108.8
C1 ⁱ —C3—C4	135.31 (19)	H9A—C9—H9B	107.6
C5—C4—C6	122.45 (19)	C9—C10—C11	112.2 (2)
C5—C4—C3	105.72 (18)	C9—C10—H10A	109.2
C6—C4—C3	131.82 (18)	C11—C10—H10A	109.2
N1—C5—O1	115.50 (19)	C9—C10—H10B	109.2
N1—C5—C4	132.4 (2)	C11—C10—H10B	109.2
O1—C5—C4	112.08 (18)	H10A—C10—H10B	107.9
O2—C6—O3	121.9 (2)	C10—C11—H11A	109.5
O2—C6—C4	124.58 (19)	C10—C11—H11B	109.5
O3—C6—C4	113.54 (18)	H11A—C11—H11B	109.5
O3—C7—C8	109.05 (16)	C10—C11—H11C	109.5
O3—C7—H7A	109.9	H11A—C11—H11C	109.5
C8—C7—H7A	109.9	H11B—C11—H11C	109.5
O3—C7—H7B	109.9	C5—N1—H1A	119.4 (15)
C8—C7—H7B	109.9	C5—N1—H1B	119.5 (15)
H7A—C7—H7B	108.3	H1A—N1—H1B	121 (2)
C7—C8—C9	110.81 (18)	C5—O1—C2	106.54 (16)
C7—C8—H8A	109.5	C6—O3—C7	115.84 (15)
C9—C8—H8A	109.5		
C3 ⁱ —C1—C2—C3	0.1 (3)	C5—C4—C6—O2	-0.8 (3)
C3 ⁱ —C1—C2—O1	179.41 (17)	C3—C4—C6—O2	178.5 (2)
C1—C2—C3—C1 ⁱ	-0.1 (3)	C5—C4—C6—O3	179.06 (18)
O1—C2—C3—C1 ⁱ	-179.49 (16)	C3—C4—C6—O3	-1.6 (3)
C1—C2—C3—C4	179.22 (19)	O3—C7—C8—C9	-178.43 (16)
O1—C2—C3—C4	-0.2 (2)	C7—C8—C9—C10	-179.49 (19)
C2—C3—C4—C5	0.7 (2)	C8—C9—C10—C11	179.2 (2)
C1 ⁱ —C3—C4—C5	179.8 (2)	N1—C5—O1—C2	-178.64 (17)
C2—C3—C4—C6	-178.7 (2)	C4—C5—O1—C2	0.8 (2)
C1 ⁱ —C3—C4—C6	0.4 (4)	C1—C2—O1—C5	-179.79 (18)
C6—C4—C5—N1	-2.1 (4)	C3—C2—O1—C5	-0.3 (2)
C3—C4—C5—N1	178.4 (2)	O2—C6—O3—C7	-0.4 (3)
C6—C4—C5—O1	178.55 (17)	C4—C6—O3—C7	179.72 (16)
C3—C4—C5—O1	-0.9 (2)	C8—C7—O3—C6	-178.24 (17)

Symmetry code: (i) $-x+1, -y, -z$.

Hydrogen-bond geometry (\AA , $^\circ$)

<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—H1A \cdots O2 ⁱⁱ	0.83 (2)	2.11 (2)	2.935 (3)	171 (2)
N1—H1B \cdots O1 ⁱⁱⁱ	0.84 (2)	2.34 (2)	3.066 (2)	144 (2)
N1—H1B \cdots O2	0.84 (2)	2.41 (2)	2.942 (3)	122.2 (18)

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