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1-[(1-Benzyl-1*H*-1,2,3-triazol-4-yl)methyl]indoline-2,3-dione

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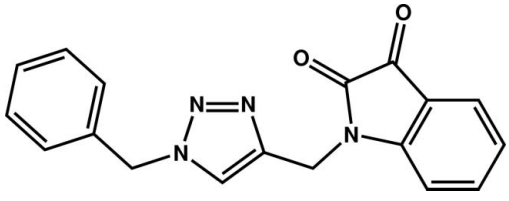
Key indicators: single-crystal X-ray study; T = 123 K; mean σ(C–C) = 0.002 Å; R factor = 0.045; wR factor = 0.123; data-to-parameter ratio = 13.3.

In the title compound, $C_{18}H_{14}N_4O_2$, the triazole ring makes dihedral angles of 77.32 (8) and 75.56 (9)°, respectively, with the indoline residue and the terminal phenyl group. In the crystal, molecules are linked by C—H···N hydrogen bonds into tapes parallel to the b axis. The tapes are linked together by π–π interactions between triazole rings [inter-centroid distance = 3.4945 (9) Å].

Related literature

For the biological activity of indoline derivatives, see: Bhrigu *et al.* (2010); Da Silva *et al.* (2001); Ramachandran (2011); Smitha *et al.* (2008). For structures of indoline-2,3-dione derivatives, see: Qachchachi *et al.* (2013, 2014).



Experimental

Crystal data

$C_{18}H_{14}N_4O_2$ M_r = 318.33
Monoclinic, $P2_1/c$
a = 11.53860 (18) Å
b = 5.38700 (9) Å
c = 23.2433 (4) Å
β = 92.1048 (16)°
V = 1443.79 (4) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 0.81 mm^{-1}
T = 123 K
0.20 × 0.04 × 0.02 mm

Data collection

Agilent SuperNova, Single source at offset, Atlas diffractometer
Absorption correction: multi-scan [*CrysAlis PRO* (Agilent, 2013), using expressions derived from Clark & Reid (1995)]
T_{min} = 0.722, T_{max} = 1.000
11043 measured reflections
2882 independent reflections
2480 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.123
S = 1.04
2882 reflections
217 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C11—H11···N2^{i}	0.93	2.50	3.383 (2)	158
C11—H11···N3^{i}	0.93	2.40	3.313 (2)	167

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

Data collection: *CrysAlis PRO* (Agilent, 2013); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *publCIF* (Westrip, 2010).

Supporting information for this paper is available from the IUCr electronic archives (Reference: BT6975).

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1-[(1-Benzyl-1*H*-1,2,3-triazol-4-yl)methyl]indoline-2,3-dione

Fatima-Zahrae Qachchachi, Youssef Kandri Rodi, El Mokhtar Essassi, Michael Bodensteiner and Lahcen El Ammari

S1. Comment

Isatin, 1*H*-indole-2,3-dione, is a heterocyclic compound of significant importance in medicinal chemistry. It is a synthetically versatile molecule, a precursor for a large number of pharmacologically active compounds. Isatin and its derivatives have aroused great attention in recent years due to their wide variety of biological activities, relevant to application as insecticides and fungicides and in a broad range of drug therapies, including anticancer drugs, antibiotics and antidepressants (Bhrigu *et al.*, 2010; Da Silva *et al.*, 2001; Ramachandran, 2011; Smitha *et al.*, 2008). As a continuation of our research work devoted to the development of isatin derivatives (Qachchachi *et al.*, 2013, 2014), we report in this paper the synthesis of a new indoline-2,3-dione derivative.

The molecule of title compound is build up from a fused five- and six-membered rings linked to a triazole ring which is connected to a benzyl ring as shown in Fig. 1. The indoline ring and the two carbonyl oxygen atoms are nearly coplanar, with the largest deviation from the mean plane being -0.059 (2) A° at O2 atom. The triazole plane is nearly perpendicular to the mean plane passing through the fused ring system (N1, C1 to C8) and to the terminal phenyl ring (C13 to C18) as indicated by the dihedral angles between them of 77.32 (8)° and 75.56 (9)°, respectively. The indazole system makes a dihedral angle of 77.02 (8)° with the phenyl ring.

In the crystal, the molecules are linked by C11–H11···N2 and C11–H11···N3 hydrogen bonds in the way to build bands parallel to the *b* axis direction. Two bands are linked together by *π*–*π* interactions between triazole rings [intercentroid distance = 3.494 Å] as shown in Fig. 2 and Table 1.

S2. Experimental

To a solution of 1-(prop-2-ynyl)indoline-2,3-dione (0.2 g, 2.4 mmol) dissolved in EtOH/H_2O (1,1) was added 1-(azidomethyl)benzene (0.4 g, 4.1 mmol), in presence of $CuSO_4$. The mixture was stirred for 24 h; the reaction was monitored by thin layer chromatography. The mixture was filtered and the solvent removed under vacuum. The solid obtained was recrystallized from ethanol to afford the title compound as yellow crystals in 81% yield.

S3. Refinement

All H atoms could be located in a difference Fourier map. Nevertheless, they were placed in calculated positions with C—H = 0.93 Å (aromatic), and C—H = 0.97 Å (methylene) and refined as riding on their parent atoms with U_{iso}(H) = 1.2 U_{eq} (aromatic and methylene).

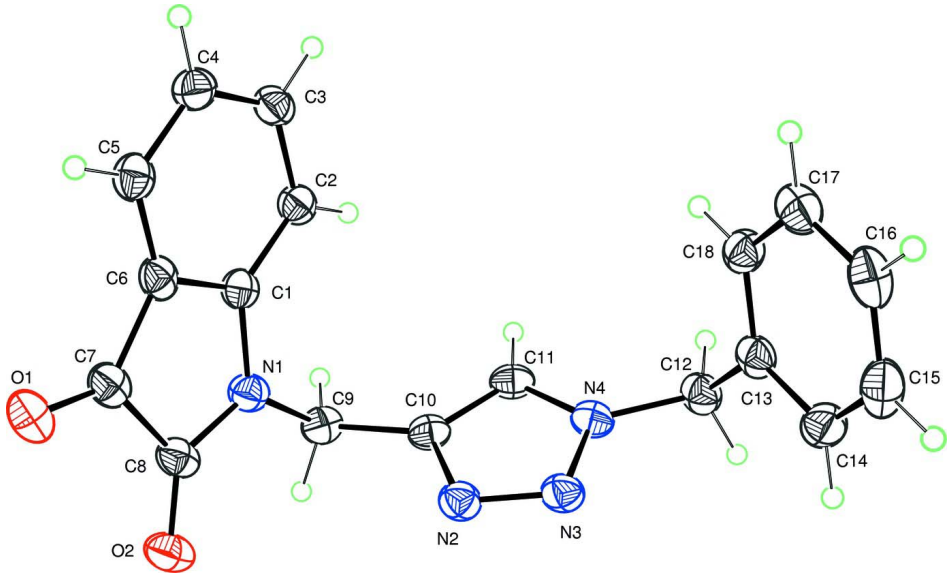

Figure 1

Molecular plot the title compound with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small circles.

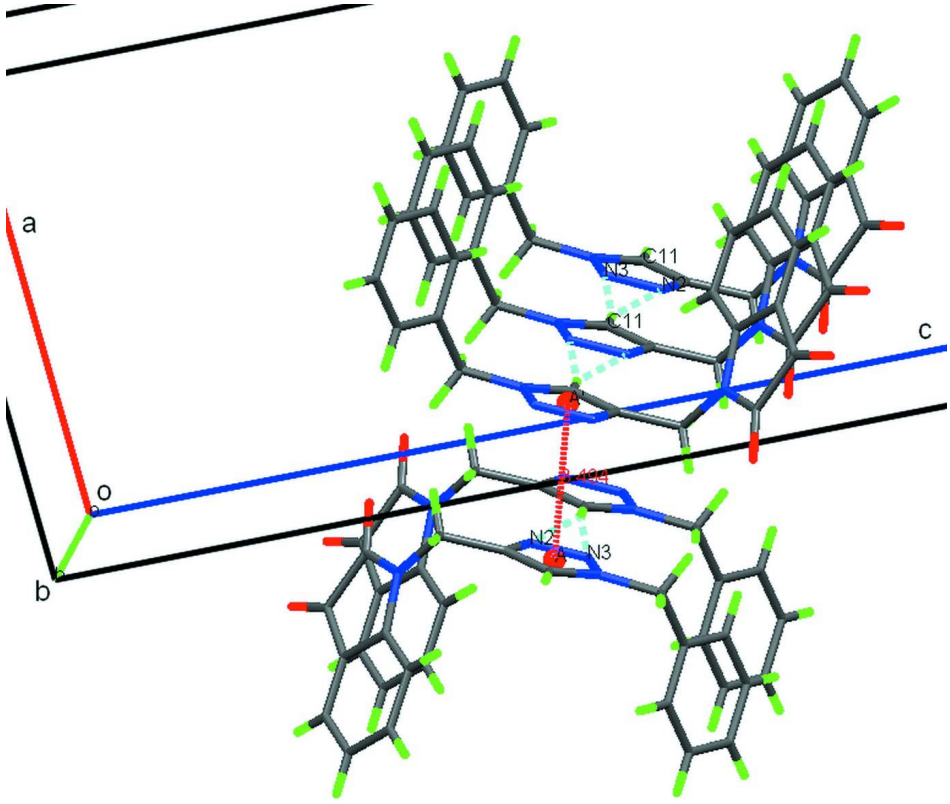

Figure 2

Intermolecular π–π (red dashed line) and hydrogen interactions (dashed blue lines) in the title compound.

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Crystal data

$C_{18}H_{14}N_4O_2$
$M_r = 318.33$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 11.53860\ (18)$ Å
$b = 5.38700\ (9)$ Å
$c = 23.2433\ (4)$ Å
$\beta = 92.1048\ (16)°$
$V = 1443.79\ (4)$ Å^3
$Z = 4$
$F(000) = 664$
$D_x = 1.464$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 4927 reflections
$\theta = 3.8–73.3°$
$\mu = 0.81$ mm^{-1}
$T = 123$ K
Rod, clear intense yellow
0.20 × 0.04 × 0.02 mm

Data collection

Agilent SuperNova, Single source at offset, Atlas diffractometer
Radiation source: SuperNova (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.3546 pixels mm^{-1}
ω scans
Absorption correction: multi-scan [*CrysAlis PRO* (Agilent, 2013), using expressions derived from Clark & Reid (1995)]
$T_{min} = 0.722$, $T_{max} = 1.000$
11043 measured reflections
2882 independent reflections
2480 reflections with $I > 2\sigma(I)$
$R_{int} = 0.032$
$\theta_{max} = 73.5°$, $\theta_{min} = 3.8°$
$h = -14\rightarrow11$
$k = -6\rightarrow6$
$l = -28\rightarrow27$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.123$
$S = 1.04$
2882 reflections
217 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
$w = 1/[\sigma^2(F_o^2) + (0.0677P)^2 + 0.6175P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.44$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-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 $F^2 > 2\sigma(F^2)$ 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
O1	0.65655 (11)	−0.1406 (2)	1.29231 (5)	0.0327 (3)

O2	0.48639 (10)	−0.1470 (2)	1.19284 (6)	0.0333 (3)
N1	0.59263 (12)	0.1979 (3)	1.16704 (6)	0.0258 (3)
N3	0.66397 (12)	−0.0542 (2)	0.99818 (6)	0.0267 (3)
N4	0.67538 (12)	0.1811 (3)	0.98001 (6)	0.0255 (3)
N2	0.61294 (12)	−0.0461 (3)	1.04795 (6)	0.0264 (3)
C9	0.52982 (14)	0.2675 (3)	1.11417 (7)	0.0269 (4)
H9A	0.5179	0.4457	1.1140	0.032*
H9B	0.4541	0.1888	1.1133	0.032*
C1	0.69237 (13)	0.3209 (3)	1.18873 (7)	0.0235 (3)
C2	0.74712 (14)	0.5253 (3)	1.16601 (7)	0.0253 (3)
H2	0.7192	0.6016	1.1324	0.030*
C4	0.88894 (14)	0.5000 (3)	1.24613 (7)	0.0287 (4)
H4	0.9552	0.5625	1.2649	0.034*
C10	0.59134 (13)	0.1956 (3)	1.06114 (7)	0.0242 (3)
C18	0.94153 (15)	0.2600 (3)	0.94699 (7)	0.0287 (4)
H18	0.9284	0.4072	0.9666	0.034*
C6	0.73451 (14)	0.2077 (3)	1.23951 (7)	0.0250 (3)
C5	0.83290 (14)	0.2949 (3)	1.26844 (7)	0.0276 (4)
H5	0.8610	0.2184	1.3020	0.033*
C13	0.84837 (15)	0.1331 (3)	0.92142 (7)	0.0267 (4)
C3	0.84634 (14)	0.6118 (3)	1.19591 (7)	0.0274 (4)
H3	0.8851	0.7488	1.1817	0.033*
C7	0.65586 (14)	0.0030 (3)	1.25238 (7)	0.0264 (4)
C12	0.72714 (15)	0.2352 (3)	0.92448 (7)	0.0293 (4)
H12A	0.7291	0.4135	0.9188	0.035*
H12B	0.6789	0.1639	0.8937	0.035*
C17	1.05397 (15)	0.1708 (4)	0.94380 (8)	0.0332 (4)
H17	1.1155	0.2578	0.9611	0.040*
C16	1.07402 (17)	−0.0482 (4)	0.91471 (8)	0.0356 (4)
H16	1.1491	−0.1094	0.9125	0.043*
C11	0.63147 (13)	0.3411 (3)	1.01791 (7)	0.0258 (3)
H11	0.6289	0.5133	1.0153	0.031*
C14	0.86952 (17)	−0.0866 (3)	0.89222 (7)	0.0327 (4)
H14	0.8082	−0.1740	0.8748	0.039*
C15	0.98220 (18)	−0.1757 (4)	0.88899 (8)	0.0376 (4)
H15	0.9958	−0.3225	0.8693	0.045*
C8	0.56440 (14)	0.0017 (3)	1.20128 (7)	0.0268 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0334 (6)	0.0294 (6)	0.0359 (7)	0.0032 (5)	0.0104 (5)	0.0061 (5)
O2	0.0274 (6)	0.0285 (6)	0.0444 (7)	−0.0058 (5)	0.0064 (5)	−0.0018 (5)
N1	0.0235 (6)	0.0253 (7)	0.0286 (7)	−0.0017 (5)	0.0023 (5)	−0.0016 (5)
N3	0.0303 (7)	0.0193 (7)	0.0307 (7)	−0.0013 (5)	0.0024 (6)	0.0006 (5)
N4	0.0250 (7)	0.0215 (7)	0.0300 (7)	−0.0017 (5)	−0.0001 (5)	0.0026 (5)
N2	0.0275 (7)	0.0220 (7)	0.0299 (7)	−0.0005 (5)	0.0026 (5)	0.0003 (5)
C9	0.0239 (7)	0.0259 (8)	0.0307 (8)	0.0012 (6)	0.0000 (6)	−0.0031 (6)

C1	0.0223 (7)	0.0236 (8)	0.0250 (7)	0.0021 (6)	0.0054 (6)	−0.0039 (6)
C2	0.0269 (8)	0.0234 (8)	0.0259 (8)	0.0001 (6)	0.0040 (6)	−0.0015 (6)
C4	0.0254 (8)	0.0318 (9)	0.0288 (8)	−0.0024 (7)	0.0018 (6)	−0.0049 (7)
C10	0.0201 (7)	0.0225 (8)	0.0298 (8)	0.0008 (6)	−0.0027 (6)	−0.0019 (6)
C18	0.0337 (9)	0.0257 (8)	0.0267 (8)	−0.0003 (7)	0.0032 (7)	−0.0006 (6)
C6	0.0256 (7)	0.0242 (8)	0.0256 (8)	0.0027 (6)	0.0076 (6)	−0.0017 (6)
C5	0.0270 (8)	0.0306 (8)	0.0255 (8)	0.0032 (6)	0.0039 (6)	−0.0014 (6)
C13	0.0323 (8)	0.0242 (8)	0.0238 (7)	−0.0008 (6)	0.0033 (6)	0.0061 (6)
C3	0.0267 (8)	0.0256 (8)	0.0303 (8)	−0.0030 (6)	0.0075 (6)	−0.0025 (6)
C7	0.0267 (8)	0.0219 (8)	0.0310 (8)	0.0030 (6)	0.0090 (6)	−0.0011 (6)
C12	0.0320 (8)	0.0292 (9)	0.0268 (8)	−0.0017 (7)	0.0010 (6)	0.0056 (7)
C17	0.0304 (9)	0.0377 (10)	0.0315 (9)	−0.0009 (7)	0.0032 (7)	0.0051 (7)
C16	0.0377 (9)	0.0379 (10)	0.0318 (9)	0.0098 (8)	0.0108 (7)	0.0092 (8)
C11	0.0239 (8)	0.0190 (7)	0.0343 (9)	0.0004 (6)	−0.0029 (6)	−0.0008 (6)
C14	0.0430 (10)	0.0266 (9)	0.0284 (8)	−0.0052 (7)	0.0022 (7)	0.0005 (7)
C15	0.0555 (12)	0.0277 (9)	0.0305 (9)	0.0063 (8)	0.0130 (8)	0.0023 (7)
C8	0.0238 (8)	0.0227 (8)	0.0343 (9)	0.0001 (6)	0.0081 (6)	−0.0024 (6)

Geometric parameters (Å, º)

O1—C7	1.208 (2)	C18—C17	1.388 (3)
O2—C8	1.216 (2)	C18—C13	1.389 (2)
N1—C8	1.370 (2)	C18—H18	0.9300
N1—C1	1.406 (2)	C6—C5	1.380 (2)
N1—C9	1.453 (2)	C6—C7	1.466 (2)
N3—N2	1.318 (2)	C5—H5	0.9300
N3—N4	1.3436 (19)	C13—C14	1.390 (2)
N4—C11	1.345 (2)	C13—C12	1.507 (2)
N4—C12	1.471 (2)	C3—H3	0.9300
N2—C10	1.362 (2)	C7—C8	1.560 (2)
C9—C10	1.496 (2)	C12—H12A	0.9700
C9—H9A	0.9700	C12—H12B	0.9700
C9—H9B	0.9700	C17—C16	1.383 (3)
C1—C2	1.384 (2)	C17—H17	0.9300
C1—C6	1.400 (2)	C16—C15	1.380 (3)
C2—C3	1.397 (2)	C16—H16	0.9300
C2—H2	0.9300	C11—H11	0.9300
C4—C3	1.387 (2)	C14—C15	1.391 (3)
C4—C5	1.390 (2)	C14—H14	0.9300
C4—H4	0.9300	C15—H15	0.9300
C10—C11	1.369 (2)		
C8—N1—C1	111.37 (14)	C4—C5—H5	120.8
C8—N1—C9	124.67 (14)	C18—C13—C14	118.74 (16)
C1—N1—C9	123.94 (14)	C18—C13—C12	120.34 (16)
N2—N3—N4	107.26 (13)	C14—C13—C12	120.91 (16)
N3—N4—C11	110.80 (13)	C4—C3—C2	122.16 (16)
N3—N4—C12	120.69 (14)	C4—C3—H3	118.9

C11—N4—C12	128.48 (14)	C2—C3—H3	118.9
N3—N2—C10	108.69 (13)	O1—C7—C6	130.68 (17)
N1—C9—C10	113.14 (13)	O1—C7—C8	124.58 (15)
N1—C9—H9A	109.0	C6—C7—C8	104.74 (13)
C10—C9—H9A	109.0	N4—C12—C13	112.11 (13)
N1—C9—H9B	109.0	N4—C12—H12A	109.2
C10—C9—H9B	109.0	C13—C12—H12A	109.2
H9A—C9—H9B	107.8	N4—C12—H12B	109.2
C2—C1—C6	121.28 (15)	C13—C12—H12B	109.2
C2—C1—N1	128.14 (15)	H12A—C12—H12B	107.9
C6—C1—N1	110.58 (14)	C16—C17—C18	119.66 (18)
C1—C2—C3	116.92 (15)	C16—C17—H17	120.2
C1—C2—H2	121.5	C18—C17—H17	120.2
C3—C2—H2	121.5	C15—C16—C17	119.75 (17)
C3—C4—C5	120.24 (16)	C15—C16—H16	120.1
C3—C4—H4	119.9	C17—C16—H16	120.1
C5—C4—H4	119.9	N4—C11—C10	105.03 (14)
N2—C10—C11	108.21 (14)	N4—C11—H11	127.5
N2—C10—C9	121.95 (15)	C10—C11—H11	127.5
C11—C10—C9	129.80 (15)	C13—C14—C15	120.10 (17)
C17—C18—C13	121.12 (17)	C13—C14—H14	120.0
C17—C18—H18	119.4	C15—C14—H14	120.0
C13—C18—H18	119.4	C16—C15—C14	120.62 (17)
C5—C6—C1	121.09 (16)	C16—C15—H15	119.7
C5—C6—C7	131.36 (16)	C14—C15—H15	119.7
C1—C6—C7	107.54 (15)	O2—C8—N1	127.25 (16)
C6—C5—C4	118.32 (16)	O2—C8—C7	127.03 (16)
C6—C5—H5	120.8	N1—C8—C7	105.70 (13)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11···N2^{i}	0.93	2.50	3.383 (2)	158
C11—H11···N3^{i}	0.93	2.40	3.313 (2)	167

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