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# 2-(1*H*-Indol-3-yl)-2′-(1*H*-indol-3-ylmethylene)acetohydrazide

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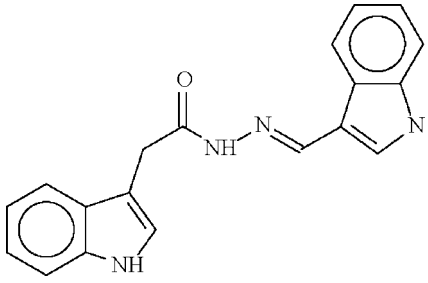
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.034; $wR$ factor = 0.100; data-to-parameter ratio = 8.3.

The molecules of the title compound, $C_{19}H_{16}N_4O$, are linked into a three-dimensional architecture by N—H···O hydrogen bonds.

## Related literature

For a related crystal structure, see Ali *et al.* (2007).




## Experimental

### Crystal data

$C_{19}H_{16}N_4O$
$M_r$ = 316.36
Monoclinic, *Cc*
$a$ = 14.0350 (2) Å
$b$ = 14.4517 (2) Å
$c$ = 8.1372 (1) Å
$\beta$ = 102.193 (1)°
$V$ = 1613.23 (4) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 293 (2) K
0.60 × 0.15 × 0.10 mm

### Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: none
12370 measured reflections
2340 independent reflections
2260 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.023

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.100
$S$ = 1.17
2340 reflections
281 parameters
17 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.38 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.26 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1N···O1$^{i}$ | 0.88 (1) | 1.98 (1) | 2.848 (2) | 174 (3) |
| N3—H3N···O1$^{ii}$ | 0.87 (1) | 1.97 (1) | 2.808 (2) | 163 (2) |

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2473).

## References

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# supplementary materials

*Acta Cryst.* (2007). E**63**, o3459 [ **doi:10.1107/S1600536807032655** ]

# 2-(1*H*-Indol-3-yl)-2'-(1*H*-indol-3-ylmethylene)acetohydrazide

**H. M. Ali, J. Nazzatush Shimar and S. W. Ng**

## Comment

A previous study reported 2'-[(5-chloro-1*H*-indol-3-yl)methylene]-2-(1*H*-indol-3-yl)acetohydrazide, a compound that is N–H···O hydrogen bonded into a three-dimensional network (Ali *et al.*, 2007). Although there are three possible donor sites, the site belonging to the indolyl ring that is linked to the methylene unit is not involved in the H bond interactions. A similar type of hydrogen bonding (Table 1) is found in the unsubstituted title compound, (I), (Fig. 1).

## Experimental

Indol-3-yl-acetylhydrazine (0.30 g, 1.6 mmol) and indol-3-ylcarboxaldehyde (0.20 g, 1.6 mmol) were heated in ethanol (50 ml) for 2 h. The solution was filtered; slow evaporation of the solvent yielded faint yellow needles of (I).

## Refinement

Anomalouse dispersion was negligible and Friedel pairs were merged before refinement. All hydrogen atoms were located in difference Fourier maps, and were refined with distance restraints C—H = 1.00±0.01 Å and N–H = 0.88±0.01 Å. Their $U_{iso}$ values were freely refined. Friedel pairs were merged.

## Figures

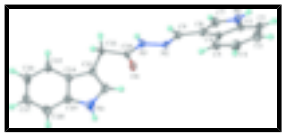

Fig. 1. View of (I) with displacement ellipsoids drawn at the 70% probability level, and H atoms as spheres of arbitrary radius.

## 2-(1*H*-Indol-3-yl)-2'-(1*H*-indol-3-ylmethylene)acetohydrazide

*Crystal data*

| | |
|---|---|
| $C_{19}H_{16}N_4O$ | $F_{000}$ = 664 |
| $M_r$ = 316.36 | $D_x$ = 1.303 Mg m$^{-3}$ |
| Monoclinic, *Cc* | Mo *K*α radiation<br>λ = 0.71073 Å |
| Hall symbol: C -2yc | Cell parameters from 8692 reflections |
| *a* = 14.0350 (2) Å | θ = 2.8–30.2º |
| *b* = 14.4517 (2) Å | μ = 0.08 mm$^{-1}$ |
| *c* = 8.1372 (1) Å | *T* = 293 (2) K |
| β = 102.193 (1)º | Tapered needle, light yellow |
| *V* = 1613.23 (4) Å$^3$ | 0.60 × 0.15 × 0.10 mm |

$Z = 4$

*Data collection*

| | |
|---|---|
| Bruker APEXII CCD area-detector diffractometer | 2260 reflections with $I > 2\sigma(I)$ |
| Radiation source: medium-focus sealed tube | $R_{int} = 0.023$ |
| Monochromator: graphite | $\theta_{max} = 30.0°$ |
| $T = 173(2)$ K | $\theta_{min} = 2.1°$ |
| φ and ω scans | $h = -19 \rightarrow 19$ |
| Absorption correction: none | $k = -20 \rightarrow 20$ |
| 12370 measured reflections | $l = -11 \rightarrow 11$ |
| 2340 independent reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full | H atoms treated by a mixture of independent and constrained refinement |
| $R[F^2 > 2\sigma(F^2)] = 0.034$ | $w = 1/[\sigma^2(F_o^2) + (0.0767P)^2 + 0.0497P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2) = 0.100$ | $(\Delta/\sigma)_{max} = 0.001$ |
| $S = 1.17$ | $\Delta\rho_{max} = 0.38$ e Å$^{-3}$ |
| 2340 reflections | $\Delta\rho_{min} = -0.26$ e Å$^{-3}$ |
| 281 parameters | Extinction correction: none |
| 17 restraints | Absolute structure: Friedel pairs were merged |
| Primary atom site location: structure-invariant direct methods | Flack parameter: ? |
| Secondary atom site location: difference Fourier map | Rogers parameter: ? |

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.50000 (8) | 0.58900 (8) | 0.50001 (14) | 0.0172 (2) |
| N1 | 0.86357 (11) | 0.22337 (10) | 0.56290 (18) | 0.0207 (3) |
| N2 | 0.62106 (9) | 0.44789 (8) | 0.44976 (15) | 0.0139 (2) |
| N3 | 0.55394 (9) | 0.49082 (9) | 0.32082 (15) | 0.0143 (2) |
| N4 | 0.20100 (11) | 0.47912 (12) | 0.2027 (2) | 0.0279 (3) |
| C1 | 0.87353 (11) | 0.28098 (11) | 0.7011 (2) | 0.0176 (3) |
| C2 | 0.94407 (13) | 0.28031 (13) | 0.8506 (2) | 0.0236 (3) |
| C3 | 0.93560 (13) | 0.34678 (13) | 0.9698 (2) | 0.0260 (3) |
| C4 | 0.85926 (14) | 0.41173 (13) | 0.9415 (2) | 0.0247 (3) |
| C5 | 0.79050 (12) | 0.41325 (11) | 0.7917 (2) | 0.0193 (3) |
| C6 | 0.79757 (10) | 0.34736 (10) | 0.66815 (18) | 0.0150 (3) |
| C7 | 0.78624 (12) | 0.25238 (12) | 0.44324 (19) | 0.0204 (3) |
| C8 | 0.74261 (11) | 0.32866 (10) | 0.50057 (19) | 0.0160 (3) |
| C9 | 0.66442 (11) | 0.37875 (10) | 0.39548 (18) | 0.0154 (3) |

| | | | | |
|---|---|---|---|---|
| C10 | 0.49922 (10) | 0.56129 (9) | 0.35533 (18) | 0.0134 (2) |
| C11 | 0.43239 (10) | 0.60328 (10) | 0.20165 (19) | 0.0152 (3) |
| C12 | 0.30093 (12) | 0.48812 (12) | 0.2490 (2) | 0.0226 (3) |
| C13 | 0.33009 (11) | 0.56780 (10) | 0.18153 (18) | 0.0154 (3) |
| C14 | 0.24281 (10) | 0.61075 (10) | 0.08736 (18) | 0.0155 (3) |
| C15 | 0.22490 (11) | 0.69156 (11) | −0.0099 (2) | 0.0193 (3) |
| C16 | 0.12907 (13) | 0.71310 (12) | −0.0859 (2) | 0.0246 (3) |
| C17 | 0.05120 (13) | 0.65631 (15) | −0.0636 (2) | 0.0274 (4) |
| C18 | 0.06691 (12) | 0.57637 (15) | 0.0317 (2) | 0.0276 (4) |
| C19 | 0.16355 (12) | 0.55390 (12) | 0.1053 (2) | 0.0212 (3) |
| H1n | 0.906 (2) | 0.1812 (18) | 0.551 (4) | 0.046 (8)* |
| H3n | 0.5469 (17) | 0.4733 (16) | 0.2169 (15) | 0.017 (5)* |
| H4n | 0.167 (2) | 0.4364 (17) | 0.242 (4) | 0.041 (8)* |
| H2 | 0.9927 (18) | 0.2299 (16) | 0.860 (4) | 0.041 (8)* |
| H3 | 0.9847 (16) | 0.348 (2) | 1.079 (2) | 0.034 (7)* |
| H4 | 0.851 (2) | 0.4539 (18) | 1.034 (3) | 0.041 (7)* |
| H5 | 0.7363 (14) | 0.4593 (15) | 0.772 (3) | 0.027 (6)* |
| H7 | 0.7666 (19) | 0.2195 (16) | 0.334 (2) | 0.026 (6)* |
| H9 | 0.6452 (19) | 0.3595 (18) | 0.2750 (15) | 0.025 (6)* |
| H11A | 0.4299 (18) | 0.6713 (7) | 0.218 (3) | 0.022 (6)* |
| H11B | 0.4619 (17) | 0.5947 (18) | 0.101 (2) | 0.024 (6)* |
| H12 | 0.341 (2) | 0.439 (2) | 0.309 (4) | 0.034 (7)* |
| H15 | 0.2789 (15) | 0.7343 (17) | −0.021 (4) | 0.032 (7)* |
| H16 | 0.117 (2) | 0.7690 (13) | −0.159 (3) | 0.037 (8)* |
| H17 | −0.0162 (10) | 0.6719 (19) | −0.124 (3) | 0.032 (7)* |
| H18 | 0.0150 (16) | 0.5337 (17) | 0.050 (4) | 0.037 (7)* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0198 (5) | 0.0187 (5) | 0.0121 (5) | 0.0055 (4) | 0.0011 (4) | −0.0006 (4) |
| N1 | 0.0239 (6) | 0.0203 (6) | 0.0181 (6) | 0.0101 (5) | 0.0049 (5) | 0.0000 (5) |
| N2 | 0.0131 (5) | 0.0155 (5) | 0.0118 (6) | 0.0026 (4) | 0.0000 (4) | 0.0025 (4) |
| N3 | 0.0158 (5) | 0.0172 (5) | 0.0088 (5) | 0.0037 (4) | 0.0001 (4) | −0.0002 (4) |
| N4 | 0.0196 (7) | 0.0330 (8) | 0.0278 (7) | −0.0075 (5) | −0.0029 (5) | 0.0127 (6) |
| C1 | 0.0175 (6) | 0.0186 (6) | 0.0167 (7) | 0.0046 (5) | 0.0034 (5) | 0.0022 (5) |
| C2 | 0.0198 (7) | 0.0287 (8) | 0.0207 (8) | 0.0060 (6) | 0.0005 (6) | 0.0044 (6) |
| C3 | 0.0236 (7) | 0.0316 (8) | 0.0187 (8) | 0.0000 (6) | −0.0046 (6) | −0.0001 (6) |
| C4 | 0.0268 (8) | 0.0263 (8) | 0.0187 (7) | −0.0013 (6) | −0.0007 (6) | −0.0057 (6) |
| C5 | 0.0210 (7) | 0.0180 (7) | 0.0181 (7) | 0.0027 (5) | 0.0022 (5) | −0.0031 (5) |
| C6 | 0.0147 (6) | 0.0151 (6) | 0.0149 (6) | 0.0029 (4) | 0.0024 (5) | 0.0006 (5) |
| C7 | 0.0244 (7) | 0.0199 (7) | 0.0163 (7) | 0.0065 (5) | 0.0033 (5) | −0.0023 (5) |
| C8 | 0.0174 (6) | 0.0157 (6) | 0.0141 (6) | 0.0040 (5) | 0.0017 (5) | −0.0001 (5) |
| C9 | 0.0163 (6) | 0.0170 (6) | 0.0122 (6) | 0.0026 (5) | 0.0009 (5) | 0.0001 (5) |
| C10 | 0.0123 (5) | 0.0147 (5) | 0.0122 (6) | 0.0014 (4) | 0.0004 (4) | 0.0024 (5) |
| C11 | 0.0141 (6) | 0.0176 (6) | 0.0125 (6) | 0.0027 (5) | −0.0005 (5) | 0.0038 (5) |
| C12 | 0.0198 (7) | 0.0254 (7) | 0.0196 (7) | −0.0031 (6) | −0.0027 (6) | 0.0074 (6) |
| C13 | 0.0150 (6) | 0.0177 (6) | 0.0123 (6) | 0.0010 (5) | −0.0001 (5) | 0.0013 (5) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C14 | 0.0149 (6) | 0.0186 (6) | 0.0121 (6) | 0.0019 (5) | 0.0010 (5) | −0.0014 (5) |
| C15 | 0.0189 (7) | 0.0195 (6) | 0.0180 (7) | 0.0048 (5) | 0.0005 (5) | 0.0001 (5) |
| C16 | 0.0222 (8) | 0.0244 (7) | 0.0246 (8) | 0.0086 (6) | −0.0010 (6) | 0.0016 (6) |
| C17 | 0.0174 (7) | 0.0389 (9) | 0.0231 (8) | 0.0073 (6) | −0.0018 (6) | −0.0001 (7) |
| C18 | 0.0157 (7) | 0.0402 (9) | 0.0250 (8) | −0.0026 (6) | −0.0001 (6) | 0.0007 (7) |
| C19 | 0.0173 (6) | 0.0279 (8) | 0.0170 (7) | −0.0019 (5) | 0.0005 (5) | 0.0032 (6) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| O1—C10 | 1.2414 (19) | C7—C8 | 1.389 (2) |
| N1—C7 | 1.362 (2) | C7—H7 | 0.996 (10) |
| N1—C1 | 1.382 (2) | C8—C9 | 1.436 (2) |
| N1—H1n | 0.876 (10) | C9—H9 | 1.000 (10) |
| N2—C9 | 1.2952 (18) | C10—C11 | 1.5220 (19) |
| N2—N3 | 1.3985 (16) | C11—C13 | 1.501 (2) |
| N3—C10 | 1.3405 (18) | C11—H11A | 0.994 (10) |
| N3—H3n | 0.868 (10) | C11—H11B | 1.000 (10) |
| N4—C19 | 1.377 (2) | C12—C13 | 1.375 (2) |
| N4—C12 | 1.379 (2) | C12—H12 | 0.97 (3) |
| N4—H4n | 0.883 (10) | C13—C14 | 1.4410 (19) |
| C1—C2 | 1.397 (2) | C14—C15 | 1.403 (2) |
| C1—C6 | 1.4171 (19) | C14—C19 | 1.415 (2) |
| C2—C3 | 1.388 (3) | C15—C16 | 1.392 (2) |
| C2—H2 | 0.991 (10) | C15—H15 | 0.996 (10) |
| C3—C4 | 1.406 (3) | C16—C17 | 1.409 (3) |
| C3—H3 | 1.002 (10) | C16—H16 | 0.998 (10) |
| C4—C5 | 1.386 (2) | C17—C18 | 1.383 (3) |
| C4—H4 | 0.993 (10) | C17—H17 | 0.994 (10) |
| C5—C6 | 1.404 (2) | C18—C19 | 1.400 (2) |
| C5—H5 | 0.998 (10) | C18—H18 | 0.991 (10) |
| C6—C8 | 1.443 (2) | | |
| C7—N1—C1 | 108.94 (12) | N2—C9—H9 | 120.0 (16) |
| C7—N1—H1n | 127 (2) | C8—C9—H9 | 117.2 (16) |
| C1—N1—H1n | 124 (2) | O1—C10—N3 | 123.58 (13) |
| C9—N2—N3 | 112.15 (12) | O1—C10—C11 | 122.08 (13) |
| C10—N3—N2 | 120.32 (12) | N3—C10—C11 | 114.31 (13) |
| C10—N3—H3n | 118.3 (16) | C13—C11—C10 | 111.28 (12) |
| N2—N3—H3n | 121.4 (16) | C13—C11—H11A | 107.0 (15) |
| C19—N4—C12 | 109.00 (14) | C10—C11—H11A | 108.4 (14) |
| C19—N4—H4n | 126 (2) | C13—C11—H11B | 114.9 (15) |
| C12—N4—H4n | 124 (2) | C10—C11—H11B | 109.4 (15) |
| N1—C1—C2 | 129.47 (15) | H11A—C11—H11B | 106 (2) |
| N1—C1—C6 | 108.12 (13) | C13—C12—N4 | 109.95 (14) |
| C2—C1—C6 | 122.40 (15) | C13—C12—H12 | 128.8 (18) |
| C3—C2—C1 | 117.02 (15) | N4—C12—H12 | 120.8 (18) |
| C3—C2—H2 | 128.1 (19) | C12—C13—C14 | 106.37 (13) |
| C1—C2—H2 | 114.8 (19) | C12—C13—C11 | 126.96 (13) |
| C2—C3—C4 | 121.48 (15) | C14—C13—C11 | 126.67 (13) |
| C2—C3—H3 | 118.9 (17) | C15—C14—C19 | 119.35 (14) |

| | | | |
|---|---|---|---|
| C4—C3—H3 | 119.6 (17) | C15—C14—C13 | 133.57 (14) |
| C5—C4—C3 | 121.32 (16) | C19—C14—C13 | 107.08 (13) |
| C5—C4—H4 | 119.3 (19) | C16—C15—C14 | 118.55 (15) |
| C3—C4—H4 | 119.2 (19) | C16—C15—H15 | 120.2 (17) |
| C4—C5—C6 | 118.54 (15) | C14—C15—H15 | 121.2 (17) |
| C4—C5—H5 | 121.0 (16) | C15—C16—C17 | 121.05 (16) |
| C6—C5—H5 | 120.4 (16) | C15—C16—H16 | 117.9 (17) |
| C5—C6—C1 | 119.21 (14) | C17—C16—H16 | 121.1 (17) |
| C5—C6—C8 | 134.37 (14) | C18—C17—C16 | 121.51 (15) |
| C1—C6—C8 | 106.42 (13) | C18—C17—H17 | 119.1 (17) |
| N1—C7—C8 | 110.21 (14) | C16—C17—H17 | 119.3 (17) |
| N1—C7—H7 | 121.4 (15) | C17—C18—C19 | 117.31 (16) |
| C8—C7—H7 | 128.4 (15) | C17—C18—H18 | 124.8 (18) |
| C7—C8—C9 | 122.39 (14) | C19—C18—H18 | 117.9 (18) |
| C7—C8—C6 | 106.28 (13) | N4—C19—C18 | 130.20 (16) |
| C9—C8—C6 | 131.06 (13) | N4—C19—C14 | 107.59 (14) |
| N2—C9—C8 | 122.73 (13) | C18—C19—C14 | 122.20 (16) |
| C9—N2—N3—C10 | 177.12 (13) | N2—N3—C10—C11 | 177.81 (12) |
| C7—N1—C1—C2 | −177.43 (18) | O1—C10—C11—C13 | −78.13 (17) |
| C7—N1—C1—C6 | 1.60 (18) | N3—C10—C11—C13 | 99.87 (15) |
| N1—C1—C2—C3 | −179.51 (17) | C19—N4—C12—C13 | −0.6 (2) |
| C6—C1—C2—C3 | 1.6 (3) | N4—C12—C13—C14 | −0.1 (2) |
| C1—C2—C3—C4 | 0.2 (3) | N4—C12—C13—C11 | 179.88 (16) |
| C2—C3—C4—C5 | −1.4 (3) | C10—C11—C13—C12 | −20.7 (2) |
| C3—C4—C5—C6 | 0.8 (3) | C10—C11—C13—C14 | 159.29 (14) |
| C4—C5—C6—C1 | 0.9 (2) | C12—C13—C14—C15 | −179.13 (17) |
| C4—C5—C6—C8 | −178.63 (17) | C11—C13—C14—C15 | 0.9 (3) |
| N1—C1—C6—C5 | 178.76 (14) | C12—C13—C14—C19 | 0.75 (17) |
| C2—C1—C6—C5 | −2.1 (2) | C11—C13—C14—C19 | −179.23 (15) |
| N1—C1—C6—C8 | −1.63 (17) | C19—C14—C15—C16 | 0.0 (2) |
| C2—C1—C6—C8 | 177.48 (15) | C13—C14—C15—C16 | 179.90 (17) |
| C1—N1—C7—C8 | −0.93 (19) | C14—C15—C16—C17 | 1.2 (2) |
| N1—C7—C8—C9 | 174.55 (14) | C15—C16—C17—C18 | −1.1 (3) |
| N1—C7—C8—C6 | −0.11 (19) | C16—C17—C18—C19 | −0.1 (3) |
| C5—C6—C8—C7 | −179.41 (17) | C12—N4—C19—C18 | −178.80 (19) |
| C1—C6—C8—C7 | 1.06 (17) | C12—N4—C19—C14 | 1.1 (2) |
| C5—C6—C8—C9 | 6.6 (3) | C17—C18—C19—N4 | −178.77 (19) |
| C1—C6—C8—C9 | −172.95 (16) | C17—C18—C19—C14 | 1.4 (3) |
| N3—N2—C9—C8 | 174.31 (13) | C15—C14—C19—N4 | 178.78 (15) |
| C7—C8—C9—N2 | 177.46 (15) | C13—C14—C19—N4 | −1.13 (18) |
| C6—C8—C9—N2 | −9.3 (3) | C15—C14—C19—C18 | −1.3 (2) |
| N2—N3—C10—O1 | −4.2 (2) | C13—C14—C19—C18 | 178.77 (16) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1N···O1$^{i}$ | 0.88 (1) | 1.98 (1) | 2.848 (2) | 174 (3) |
| N3—H3N···O1$^{ii}$ | 0.87 (1) | 1.97 (1) | 2.808 (2) | 163 (2) |

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

**Fig. 1**