

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

N'-(2-Hydroxy-5-nitrobenzylidene)-2-(1*H*-indol-3-yl)acetohydrazide

 Subramaniam Puvaneswary, Hapipah M. Ali,
Ward T. Robinson and Seik Weng Ng*

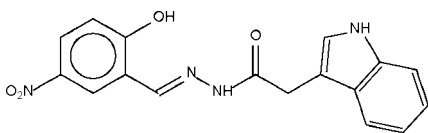
 Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

Received 10 July 2008; accepted 12 August 2008

 Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å;
 R factor = 0.045; wR factor = 0.160; data-to-parameter ratio = 16.1.

The molecule of the title compound, $\text{C}_{17}\text{H}_{14}\text{N}_4\text{O}_4$, uses its amide $-\text{NH}-$ group to form a hydrogen bond to the amido $-\text{C}(=\text{O})-$ group of an adjacent molecule to furnish a linear chain structure. The hydroxy group forms an intramolecular hydrogen bond; the indolyl $-\text{NH}-$ unit does not engage in any strong hydrogen-bonding interactions.

Related literature

 For similar compounds, see: Martin Reyes *et al.* (1986); Martin Zarza *et al.* (1989).


Experimental

Crystal data

 $\text{C}_{17}\text{H}_{14}\text{N}_4\text{O}_4$
 $M_r = 338.32$
Orthorhombic, *Pbca*
 $a = 9.5387$ (2) Å
 $b = 11.2724$ (3) Å
 $c = 29.7796$ (7) Å

 $V = 3202.0$ (1) Å³
 $Z = 8$
Mo $K\alpha$ radiation
 $\mu = 0.10$ mm⁻¹
 $T = 100$ (2) K
0.30 × 0.25 × 0.20 mm

Data collection

 Bruker SMART APEX
diffractometer
Absorption correction: none
47721 measured reflections

 3679 independent reflections
2059 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.052$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.160$
 $S = 1.02$
3679 reflections

 228 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.17$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.21$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|-----------------------------------------|-------|-------------|-------------|---------------|
| $\text{O1}-\text{H1}o\cdots\text{N2}$ | 0.84 | 1.85 | 2.583 (2) | 146 |
| $\text{N3}-\text{H3}n\cdots\text{O4}^i$ | 0.88 | 2.07 | 2.827 (2) | 144 |

 Symmetry code: (i) $x - \frac{1}{2}, y, -z + \frac{3}{2}$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINTE* (Bruker, 2007); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2008).

We thank the Science Fund (12-02-03-2031, 12-02-03-2051) and the University of Malaya (PJP) for supporting this study. We are grateful to the University of Malaya for the purchase of the diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2091).

References

- Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2007). *APEX2* and *SAINTE*. Bruker AXS Inc., Madison, Wisconsin, USA.
Martin Reyes, M. G., Gili, P., Zarza, P. M., Medina Ortega, A. & Diaz Gonzalez, M. C. (1986). *Inorg. Chim. Acta*, **116**, 153–156.
Martin Zarza, P., Gili, P., Mederos, A. & Medina, A. (1989). *Thermochim. Acta*, **156**, 231–238.
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
Westrip, S. P. (2008). *publCIF*. In preparation.

supplementary materials

Acta Cryst. (2008). E64, o1777 [doi:10.1107/S1600536808026044]

***N'*-(2-Hydroxy-5-nitrobenzylidene)-2-(1*H*-indol-3-yl)acetohydrazide**

S. Puvaneswary, H. M. Ali, W. T. Robinson and S. W. Ng

Comment

There are many examples of Schiff bases derived from the condensation of salicylaldehyde and substituted salicylaldehydes with hydrazides such as the ones reported by Martin Reyes *et al.* (1986) and Martin Zarza *et al.* (1989). The title compound (Fig. 1) is another example. The molecule uses its amido –NH– group to form a hydrogen bond to the amido –C(=O)– group of an adjacent molecule to furnish a linear chain structure.

Experimental

The Schiff base was prepared by refluxing a solution of indole-3-acetic acid hydrazide (0.34 g, 1.80 mmol) and 5-nitrosalicylaldehyde (0.30 g, 1.80 mmol) in acidified ethanol (25 ml) for 2 h. On cooling to room temperature, yellow crystals separated out.

Refinement

All H-atoms were placed in calculated positions (C—H 0.95, N—H 0.88, O—H 0.84 Å) and were included in the refinement in the riding model approximation, with $U(H)$ set to 1.2 to 1.5 $U_{eq}(C,N,O)$.

Figures

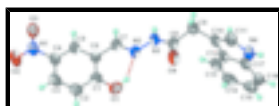


Fig. 1. Thermal ellipsoid plot of (I) (Barbour, 2001) at the 50% probability level. Dashed line indicates H-bonding.

***N'*-(2-Hydroxy-5-nitrobenzylidene)-2-(1*H*-indol-3-yl)acetohydrazide**

Crystal data

C₁₇H₁₄N₄O₄

$M_r = 338.32$

Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

$a = 9.5387$ (2) Å

$b = 11.2724$ (3) Å

$c = 29.7796$ (7) Å

$V = 3202.0$ (1) Å³

$Z = 8$

$F_{000} = 1408$

$D_x = 1.404$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 3679 reflections

$\theta = 2.5$ – 22.2°

$\mu = 0.10$ mm⁻¹

$T = 100$ (2) K

Irregular block, yellow

0.30 × 0.25 × 0.20 mm

supplementary materials

Data collection

| | |
|------------------------------------------|----------------------------------------|
| Bruker SMART APEX diffractometer | 2059 reflections with $I > 2\sigma(I)$ |
| Radiation source: fine-focus sealed tube | $R_{\text{int}} = 0.053$ |
| Monochromator: graphite | $\theta_{\text{max}} = 27.5^\circ$ |
| $T = 100(2)$ K | $\theta_{\text{min}} = 1.4^\circ$ |
| ω scans | $h = -12 \rightarrow 12$ |
| Absorption correction: None | $k = -14 \rightarrow 13$ |
| 47721 measured reflections | $l = -38 \rightarrow 38$ |
| 3679 independent reflections | |

Refinement

| | |
|----------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------|
| Refinement on F^2 | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full | H-atom parameters constrained |
| $R[F^2 > 2\sigma(F^2)] = 0.044$ | $w = 1/[\sigma^2(F_o^2) + (0.0885P)^2]$ |
| $wR(F^2) = 0.160$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.02$ | $(\Delta/\sigma)_{\text{max}} = 0.001$ |
| 3679 reflections | $\Delta\rho_{\text{max}} = 0.18 \text{ e } \text{\AA}^{-3}$ |
| 228 parameters | $\Delta\rho_{\text{min}} = -0.21 \text{ e } \text{\AA}^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: SHELXL97 (Sheldrick, 2008), $F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$ |
| Secondary atom site location: difference Fourier map | Extinction coefficient: 0.007 (1) |

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.

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

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|--------------|-------------|----------------------------------|
| O1 | 0.76143 (16) | 0.34962 (15) | 0.66810 (5) | 0.0747 (5) |
| H1O | 0.7344 | 0.4058 | 0.6845 | 0.112* |
| O2 | 0.50825 (18) | 0.27110 (16) | 0.47819 (5) | 0.0896 (6) |
| O3 | 0.36688 (19) | 0.40496 (16) | 0.50246 (5) | 0.0853 (5) |
| O4 | 0.78329 (15) | 0.61201 (15) | 0.75230 (5) | 0.0790 (5) |
| N1 | 0.4670 (2) | 0.33901 (17) | 0.50757 (6) | 0.0647 (5) |
| N2 | 0.60812 (15) | 0.52866 (14) | 0.69094 (5) | 0.0522 (4) |
| N3 | 0.56843 (16) | 0.61209 (15) | 0.72184 (5) | 0.0543 (5) |
| H3N | 0.4821 | 0.6397 | 0.7223 | 0.065* |

| | | | | |
|-----|--------------|--------------|-------------|------------|
| N4 | 0.79603 (19) | 0.75966 (17) | 0.89103 (6) | 0.0712 (5) |
| H4N | 0.8598 | 0.7879 | 0.9095 | 0.085* |
| C1 | 0.6858 (2) | 0.34823 (18) | 0.63004 (7) | 0.0563 (5) |
| C2 | 0.7229 (2) | 0.26733 (18) | 0.59698 (8) | 0.0651 (6) |
| H2 | 0.7980 | 0.2137 | 0.6022 | 0.078* |
| C3 | 0.6523 (2) | 0.26386 (18) | 0.55689 (7) | 0.0625 (6) |
| H3 | 0.6787 | 0.2090 | 0.5342 | 0.075* |
| C4 | 0.5426 (2) | 0.34134 (17) | 0.55005 (6) | 0.0538 (5) |
| C5 | 0.5011 (2) | 0.42048 (16) | 0.58253 (6) | 0.0511 (5) |
| H5 | 0.4237 | 0.4715 | 0.5772 | 0.061* |
| C6 | 0.57211 (19) | 0.42584 (16) | 0.62300 (6) | 0.0473 (5) |
| C7 | 0.53086 (19) | 0.51242 (17) | 0.65658 (6) | 0.0505 (5) |
| H7 | 0.4468 | 0.5567 | 0.6530 | 0.061* |
| C8 | 0.6644 (2) | 0.65087 (18) | 0.75150 (6) | 0.0555 (5) |
| C9 | 0.6133 (2) | 0.7485 (2) | 0.78219 (6) | 0.0643 (6) |
| H9A | 0.6427 | 0.8262 | 0.7699 | 0.077* |
| H9B | 0.5095 | 0.7472 | 0.7832 | 0.077* |
| C10 | 0.6695 (2) | 0.73543 (17) | 0.82885 (6) | 0.0546 (5) |
| C11 | 0.7735 (2) | 0.7979 (2) | 0.84821 (7) | 0.0684 (6) |
| H11 | 0.8242 | 0.8600 | 0.8340 | 0.082* |
| C12 | 0.62245 (19) | 0.65262 (16) | 0.86168 (7) | 0.0514 (5) |
| C13 | 0.5173 (2) | 0.56695 (18) | 0.86298 (8) | 0.0626 (6) |
| H13 | 0.4599 | 0.5530 | 0.8374 | 0.075* |
| C14 | 0.4978 (3) | 0.50326 (19) | 0.90151 (9) | 0.0745 (7) |
| H14 | 0.4262 | 0.4447 | 0.9024 | 0.089* |
| C15 | 0.5803 (3) | 0.5221 (2) | 0.93952 (8) | 0.0753 (7) |
| H15 | 0.5640 | 0.4760 | 0.9657 | 0.090* |
| C16 | 0.6847 (2) | 0.6062 (2) | 0.93974 (7) | 0.0667 (6) |
| H16 | 0.7411 | 0.6194 | 0.9655 | 0.080* |
| C17 | 0.7037 (2) | 0.67047 (18) | 0.90073 (7) | 0.0561 (5) |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|----|-------------|-------------|-------------|--------------|-------------|--------------|
| O1 | 0.0634 (10) | 0.0901 (11) | 0.0707 (10) | 0.0201 (8) | -0.0089 (8) | 0.0030 (8) |
| O2 | 0.0991 (14) | 0.1023 (13) | 0.0672 (11) | -0.0122 (10) | 0.0139 (9) | -0.0333 (10) |
| O3 | 0.0835 (12) | 0.0954 (12) | 0.0771 (11) | 0.0045 (10) | -0.0245 (9) | -0.0215 (9) |
| O4 | 0.0393 (9) | 0.1232 (13) | 0.0745 (11) | 0.0156 (8) | -0.0106 (7) | -0.0360 (9) |
| N1 | 0.0663 (12) | 0.0712 (12) | 0.0566 (11) | -0.0201 (10) | 0.0062 (9) | -0.0134 (10) |
| N2 | 0.0406 (9) | 0.0683 (10) | 0.0477 (9) | -0.0033 (8) | 0.0012 (7) | -0.0058 (8) |
| N3 | 0.0360 (8) | 0.0762 (11) | 0.0507 (10) | 0.0042 (8) | 0.0002 (7) | -0.0134 (8) |
| N4 | 0.0664 (12) | 0.0860 (13) | 0.0612 (11) | -0.0182 (10) | -0.0085 (9) | -0.0171 (10) |
| C1 | 0.0460 (11) | 0.0607 (12) | 0.0623 (13) | -0.0011 (9) | 0.0046 (10) | 0.0044 (10) |
| C2 | 0.0548 (13) | 0.0590 (13) | 0.0814 (16) | 0.0065 (10) | 0.0103 (12) | 0.0004 (11) |
| C3 | 0.0592 (14) | 0.0557 (12) | 0.0724 (15) | -0.0079 (10) | 0.0201 (12) | -0.0112 (10) |
| C4 | 0.0512 (12) | 0.0533 (11) | 0.0568 (12) | -0.0139 (9) | 0.0058 (10) | -0.0048 (9) |
| C5 | 0.0460 (11) | 0.0536 (11) | 0.0536 (11) | -0.0039 (9) | 0.0030 (8) | -0.0029 (9) |
| C6 | 0.0409 (10) | 0.0498 (10) | 0.0513 (11) | -0.0052 (8) | 0.0050 (8) | 0.0011 (9) |

supplementary materials

| | | | | | | |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| C7 | 0.0416 (11) | 0.0583 (11) | 0.0515 (11) | -0.0014 (9) | 0.0018 (9) | -0.0006 (9) |
| C8 | 0.0428 (12) | 0.0750 (13) | 0.0488 (11) | 0.0012 (10) | -0.0009 (9) | -0.0068 (10) |
| C9 | 0.0573 (13) | 0.0742 (14) | 0.0613 (13) | 0.0078 (11) | -0.0020 (10) | -0.0119 (11) |
| C10 | 0.0496 (12) | 0.0617 (12) | 0.0524 (11) | -0.0006 (9) | 0.0004 (9) | -0.0154 (9) |
| C11 | 0.0671 (15) | 0.0730 (14) | 0.0650 (14) | -0.0150 (12) | 0.0039 (11) | -0.0092 (11) |
| C12 | 0.0443 (11) | 0.0532 (11) | 0.0568 (12) | 0.0047 (9) | 0.0009 (9) | -0.0189 (9) |
| C13 | 0.0534 (13) | 0.0564 (12) | 0.0781 (15) | -0.0004 (10) | -0.0012 (11) | -0.0154 (11) |
| C14 | 0.0665 (15) | 0.0541 (12) | 0.103 (2) | -0.0025 (11) | 0.0122 (14) | -0.0064 (13) |
| C15 | 0.0858 (18) | 0.0594 (13) | 0.0808 (17) | 0.0180 (13) | 0.0207 (14) | 0.0039 (12) |
| C16 | 0.0717 (15) | 0.0718 (14) | 0.0566 (13) | 0.0192 (13) | -0.0007 (11) | -0.0090 (11) |
| C17 | 0.0523 (12) | 0.0578 (12) | 0.0583 (12) | 0.0059 (10) | 0.0013 (10) | -0.0171 (10) |

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

| | | | |
|------------|-------------|-------------|-------------|
| O1—C1 | 1.344 (2) | C5—H5 | 0.9500 |
| O1—H1O | 0.8400 | C6—C7 | 1.452 (3) |
| O2—N1 | 1.227 (2) | C7—H7 | 0.9500 |
| O3—N1 | 1.220 (2) | C8—C9 | 1.512 (3) |
| O4—C8 | 1.216 (2) | C9—C10 | 1.497 (3) |
| N1—C4 | 1.456 (3) | C9—H9A | 0.9900 |
| N2—C7 | 1.274 (2) | C9—H9B | 0.9900 |
| N2—N3 | 1.369 (2) | C10—C11 | 1.347 (3) |
| N3—C8 | 1.345 (2) | C10—C12 | 1.424 (3) |
| N3—H3N | 0.8800 | C11—H11 | 0.9500 |
| N4—C11 | 1.363 (3) | C12—C13 | 1.393 (3) |
| N4—C17 | 1.367 (3) | C12—C17 | 1.412 (3) |
| N4—H4N | 0.8800 | C13—C14 | 1.366 (3) |
| C1—C2 | 1.388 (3) | C13—H13 | 0.9500 |
| C1—C6 | 1.409 (3) | C14—C15 | 1.395 (3) |
| C2—C3 | 1.371 (3) | C14—H14 | 0.9500 |
| C2—H2 | 0.9500 | C15—C16 | 1.375 (3) |
| C3—C4 | 1.378 (3) | C15—H15 | 0.9500 |
| C3—H3 | 0.9500 | C16—C17 | 1.381 (3) |
| C4—C5 | 1.374 (3) | C16—H16 | 0.9500 |
| C5—C6 | 1.384 (3) | | |
| C1—O1—H1O | 109.5 | O4—C8—C9 | 123.48 (18) |
| O3—N1—O2 | 122.85 (19) | N3—C8—C9 | 114.46 (18) |
| O3—N1—C4 | 119.01 (18) | C10—C9—C8 | 111.95 (17) |
| O2—N1—C4 | 118.1 (2) | C10—C9—H9A | 109.2 |
| C7—N2—N3 | 118.59 (16) | C8—C9—H9A | 109.2 |
| C8—N3—N2 | 118.45 (16) | C10—C9—H9B | 109.2 |
| C8—N3—H3N | 120.8 | C8—C9—H9B | 109.2 |
| N2—N3—H3N | 120.8 | H9A—C9—H9B | 107.9 |
| C11—N4—C17 | 109.21 (17) | C11—C10—C12 | 106.33 (18) |
| C11—N4—H4N | 125.4 | C11—C10—C9 | 127.6 (2) |
| C17—N4—H4N | 125.4 | C12—C10—C9 | 126.11 (18) |
| O1—C1—C2 | 117.97 (19) | C10—C11—N4 | 110.5 (2) |
| O1—C1—C6 | 122.12 (18) | C10—C11—H11 | 124.7 |
| C2—C1—C6 | 119.91 (19) | N4—C11—H11 | 124.7 |

| | | | |
|--------------|--------------|-----------------|--------------|
| C3—C2—C1 | 120.8 (2) | C13—C12—C17 | 118.12 (19) |
| C3—C2—H2 | 119.6 | C13—C12—C10 | 134.45 (19) |
| C1—C2—H2 | 119.6 | C17—C12—C10 | 107.40 (17) |
| C2—C3—C4 | 118.89 (19) | C14—C13—C12 | 119.1 (2) |
| C2—C3—H3 | 120.6 | C14—C13—H13 | 120.5 |
| C4—C3—H3 | 120.6 | C12—C13—H13 | 120.5 |
| C5—C4—C3 | 121.73 (19) | C13—C14—C15 | 121.7 (2) |
| C5—C4—N1 | 118.73 (19) | C13—C14—H14 | 119.2 |
| C3—C4—N1 | 119.54 (18) | C15—C14—H14 | 119.2 |
| C4—C5—C6 | 120.04 (18) | C16—C15—C14 | 121.2 (2) |
| C4—C5—H5 | 120.0 | C16—C15—H15 | 119.4 |
| C6—C5—H5 | 120.0 | C14—C15—H15 | 119.4 |
| C5—C6—C1 | 118.63 (17) | C15—C16—C17 | 116.9 (2) |
| C5—C6—C7 | 119.78 (17) | C15—C16—H16 | 121.5 |
| C1—C6—C7 | 121.58 (18) | C17—C16—H16 | 121.5 |
| N2—C7—C6 | 119.53 (17) | N4—C17—C16 | 130.4 (2) |
| N2—C7—H7 | 120.2 | N4—C17—C12 | 106.52 (18) |
| C6—C7—H7 | 120.2 | C16—C17—C12 | 123.1 (2) |
| O4—C8—N3 | 122.03 (18) | | |
| C7—N2—N3—C8 | -163.35 (18) | N3—C8—C9—C10 | 142.14 (19) |
| O1—C1—C2—C3 | -178.10 (19) | C8—C9—C10—C11 | 103.7 (2) |
| C6—C1—C2—C3 | 1.7 (3) | C8—C9—C10—C12 | -76.0 (3) |
| C1—C2—C3—C4 | -0.7 (3) | C12—C10—C11—N4 | 0.4 (2) |
| C2—C3—C4—C5 | -0.9 (3) | C9—C10—C11—N4 | -179.39 (19) |
| C2—C3—C4—N1 | 179.78 (17) | C17—N4—C11—C10 | -0.8 (2) |
| O3—N1—C4—C5 | -1.9 (3) | C11—C10—C12—C13 | 177.9 (2) |
| O2—N1—C4—C5 | 177.32 (17) | C9—C10—C12—C13 | -2.4 (3) |
| O3—N1—C4—C3 | 177.38 (18) | C11—C10—C12—C17 | 0.1 (2) |
| O2—N1—C4—C3 | -3.4 (3) | C9—C10—C12—C17 | 179.90 (18) |
| C3—C4—C5—C6 | 1.6 (3) | C17—C12—C13—C14 | -0.6 (3) |
| N1—C4—C5—C6 | -179.14 (16) | C10—C12—C13—C14 | -178.1 (2) |
| C4—C5—C6—C1 | -0.5 (3) | C12—C13—C14—C15 | 0.1 (3) |
| C4—C5—C6—C7 | 177.88 (16) | C13—C14—C15—C16 | 0.2 (3) |
| O1—C1—C6—C5 | 178.74 (17) | C14—C15—C16—C17 | -0.1 (3) |
| C2—C1—C6—C5 | -1.0 (3) | C11—N4—C17—C16 | -178.7 (2) |
| O1—C1—C6—C7 | 0.3 (3) | C11—N4—C17—C12 | 0.8 (2) |
| C2—C1—C6—C7 | -179.43 (17) | C15—C16—C17—N4 | 179.0 (2) |
| N3—N2—C7—C6 | 178.97 (15) | C15—C16—C17—C12 | -0.4 (3) |
| C5—C6—C7—N2 | -170.09 (17) | C13—C12—C17—N4 | -178.75 (16) |
| C1—C6—C7—N2 | 8.3 (3) | C10—C12—C17—N4 | -0.6 (2) |
| N2—N3—C8—O4 | -1.8 (3) | C13—C12—C17—C16 | 0.8 (3) |
| N2—N3—C8—C9 | 176.17 (17) | C10—C12—C17—C16 | 178.93 (18) |
| O4—C8—C9—C10 | -39.9 (3) | | |

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> |
|---------------------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| O1—H1 _o \cdots N2 | 0.84 | 1.85 | 2.583 (2) | 146 |
| N3—H3 _n \cdots O4 ⁱ | 0.88 | 2.07 | 2.827 (2) | 144 |

supplementary materials

N4—H4n···O2ⁱⁱ 0.88 2.49 3.216 (2) 140
Symmetry codes: (i) $x-1/2, y, -z+3/2$; (ii) $-x+3/2, -y+1, z+1/2$.

Fig. 1

