

Pyrrole-2-carbaldehyde isonicotinoyl-hydrazone monohydrate redetermined at 120 K

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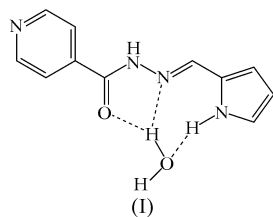
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In the title compound, $C_{11}H_{10}N_4O \cdot H_2O$, there are five independent hydrogen bonds, of $O-H \cdots O$, $O-H \cdots N$ and $N-H \cdots O$ types, which link the components into complex sheets parallel to (001).

Comment

As part of a study of isonicotinoylhydrazones, we have investigated the title compound, (I). The structure of this monohydrate was recently reported based on diffraction data collected at ambient temperature (Safoklov *et al.*, 2002), and it is clear from the unit-cell dimensions and space group that no phase change has occurred between ambient temperature and 120 K. The authors identified five independent hydrogen bonds in the structure but, although the coordinates of the H atoms were all refined, no s.u. values were quoted for the hydrogen-bond parameters and the symmetry-equivalent components involved in the hydrogen bonds were not identified. Similarly, the resulting supramolecular structure was not analysed in detail and, in particular, its dimensionality was not



specified. We have now taken the opportunity to redetermine the structure of compound (I) using diffraction data collected at 120 K, and we report here a full descriptive analysis of the supramolecular structure thus established.

Within the substituted hydrazone component, there is a clear distinction between single and double bonds (Table 1) within the spacer unit between the rings. This unit adopts an all-*trans* configuration. In the pyrrole ring, however, the C—C distances vary rather little, consistent with the aromatic character of this ring. The intrachain bond angles in the spacer unit are all well below 120° , while the torsion angles indicate near planarity of the molecule, apart from the pyridyl ring, which is rotated significantly out of the plane of the rest of the molecule, possibly driven by repulsive interactions between the H atoms bonded to atoms C13 and N17 (Fig. 1). Molecules of the organic component of (I) have no internal symmetry and hence are chiral and, in the absence of inversion twinning, each crystal will contain only one enantiomer.

There are five hydrogen bonds in the structure of (I), two each of the $O-H \cdots O$ and $N-H \cdots O$ types and one of the

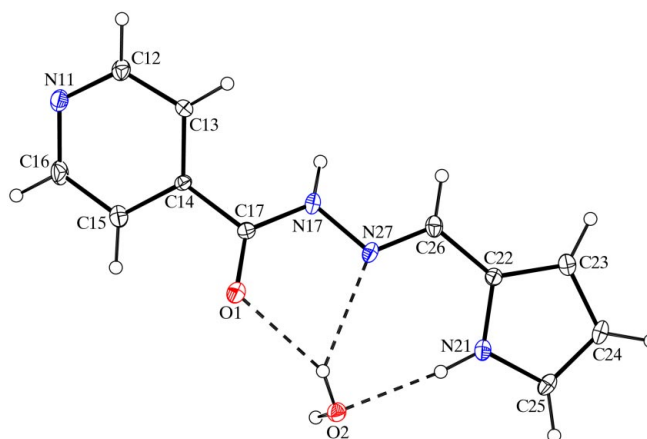


Figure 1

The independent molecular components of (I), showing the atom-labelling scheme and the hydrogen bonds within the selected asymmetric unit (dashed lines). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

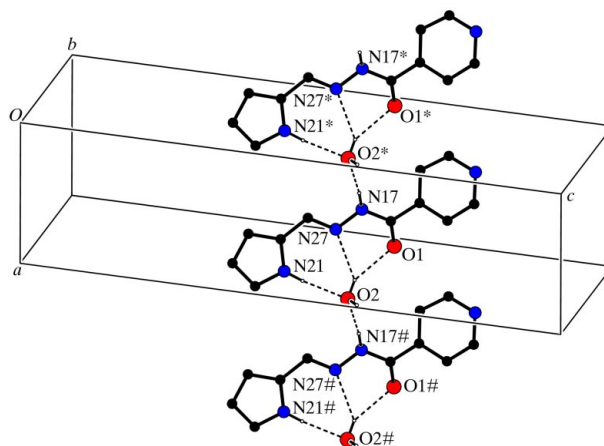
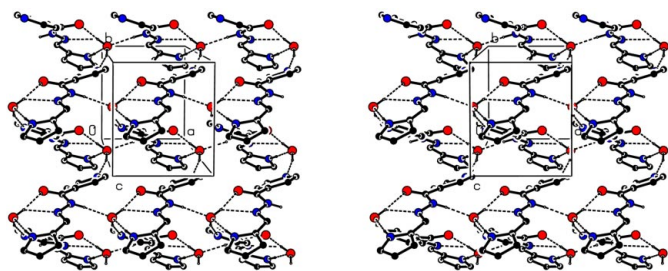


Figure 2

Part of the crystal structure of (I), showing the formation of a chain of rings along [100]. For the sake of clarity, H atoms bonded to C atoms have been omitted. Atoms marked with an asterisk (*) or a hash (#) are at the symmetry positions $(-1 + x, y, z)$ and $(1 + x, y, z)$, respectively.


Figure 3

A stereoview of part of the crystal structure of (I), showing the formation of an (001) sheet by the combination of [100] and [010] chains. For the sake of clarity, H atoms bonded to C atoms have been omitted.

O—H...O type (Table 2). Three of these occur within the selected asymmetric unit (Fig. 1), such that the water molecule is effectively tethered to the organic component. The three-centre O—H...N(O) system involving atom H2A is almost planar. There are thus two hydrogen bonds available to link these two-molecule aggregates, and the resulting sheet structure is readily analysed in terms of two independent one-dimensional substructures.

Amide atom N17 at (x, y, z) acts as a hydrogen-bond donor to water atom O2 at $(-1 + x, y, z)$, so generating by translation a $C_2^2(5)[R_1^2(5)][R_2^2(7)]$ chain of rings (Bernstein *et al.*, 1995) running parallel to the [100] direction (Fig. 2). In addition, water atom O2 at (x, y, z) acts as hydrogen-bond donor to pyridyl atom N11 at $(1 - x, -\frac{1}{2} + y, \frac{3}{2} - z)$, so forming a $C_2^2(9)$ chain running parallel to the [010] direction and generated by the 2_1 screw axis along $(\frac{1}{2}, y, \frac{3}{4})$ (Fig. 3). Water atom O2 thus acts both as a double acceptor and as a triple donor of hydrogen bonds.

The combination of these two rather elaborate substructures then generates a complex and deeply puckered (001) sheet (Fig. 3) lying in the domain $0.41 < z < 1.09$ and containing $R_6^6(23)$ rings, in addition to the $R_1^2(5)$ and $R_2^2(7)$ rings within the asymmetric unit (Fig. 1). A second similar sheet, generated by the 2_1 axes at $z = \frac{1}{4}$, lies in the domain $-0.09 < z < 0.59$. However, there are no direction-specific interactions between adjacent sheets. In particular, $X-H \cdots \pi(\text{pyridine})$ and $X-H \cdots \pi(\text{pyrrole})$ hydrogen bonds ($X = \text{O, N or C}$) and $\pi-\pi$ stacking interactions are all absent.

Experimental

Equimolar quantities (2 mmol) of pyrrole-2-carbaldehyde and isoniazid (isonicotinoylhydrazine) in tetrahydrofuran (20 ml) were heated under reflux under a dinitrogen atmosphere for 6 h. The resulting mixture was then concentrated under reduced pressure and the residue was purified by column chromatography on silica gel, eluting with a hexane–ethyl acetate gradient. Recrystallization from ethanol provided crystals of the title compound suitable for single-crystal X-ray diffraction (yield 78%, m.p. 507–509 K). MS (m/z): 214 (M^+). ^1H NMR (DMSO- d_6): δ 11.78 (1H, s, NH), 11.64 (1H, s, NH), 8.78 (2H, d, $J = 5.5$ Hz), 8.31 (1H, s, C=N–H), 7.82 (2H, d, $J = 5.5$ Hz), 6.96 (1H, s), 6.55 (1H, s), 6.17 (1H, d, $J = 2.5$ Hz); ^{13}C NMR

(DMSO- d_6): δ 160.9, 150.2, 141.8, 140.7, 126.6, 122.9, 121.4, 113.9, 109.3; IR (KBr, ν , cm^{-1}): 3213 (NH), 1647 (CO).

Crystal data

$C_{11}H_{10}N_4O \cdot H_2O$
 $M_r = 232.25$
 Orthorhombic, $P2_12_12_1$
 $a = 6.4224$ (3) Å
 $b = 7.2115$ (5) Å
 $c = 23.6073$ (16) Å
 $V = 1093.38$ (12) Å³
 $Z = 4$
 $D_x = 1.411$ Mg m⁻³

Mo $K\alpha$ radiation
 Cell parameters from 1237 reflections
 $\theta = 3.0$ – 26.5°
 $\mu = 0.10$ mm⁻¹
 $T = 120$ (2) K
 Needle, yellow
 $0.44 \times 0.06 \times 0.06$ mm

Data collection

Nonius KappaCCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
 $T_{\min} = 0.967$, $T_{\max} = 0.994$
 5095 measured reflections

1279 independent reflections
 1157 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.054$
 $\theta_{\max} = 26.5^\circ$
 $h = -7 \rightarrow 7$
 $k = -8 \rightarrow 8$
 $l = -17 \rightarrow 29$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.054$
 $wR(F^2) = 0.148$
 $S = 1.17$
 1279 reflections
 155 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0372P)^2 + 2.0901P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.35$ e Å⁻³
 $\Delta\rho_{\min} = -0.41$ e Å⁻³
 Extinction correction: SHELXL97 (Sheldrick, 1997)
 Extinction coefficient: 0.031 (6)

Table 1

Selected geometric parameters (Å, °).

C14–C17	1.497 (6)	N21–C22	1.365 (6)
C17–N17	1.345 (5)	C22–C23	1.393 (6)
N17–N27	1.393 (5)	C23–C24	1.397 (7)
N27–C26	1.289 (5)	C24–C25	1.382 (7)
C26–C22	1.442 (6)	C25–N21	1.366 (5)
C14–C17–N17	116.8 (4)	N17–N27–C26	116.5 (4)
C17–N17–N27	116.2 (4)	N27–C26–C22	117.9 (4)
C13–C14–C17–N17	–32.6 (6)	N17–N27–C26–C22	–172.1 (4)
C14–C17–N17–N27	–169.2 (4)	N27–C26–C22–C23	179.3 (4)
C17–N17–N27–C26	–178.9 (4)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O2–H2A...O1	0.84	2.18	2.934 (5)	150
O2–H2A...N27	0.84	2.38	3.011 (5)	133
N21–H21...O2	0.88	2.07	2.950 (5)	174
N17–H17...O2 ⁱ	0.88	1.95	2.822 (5)	173
O2–H2B...N11 ⁱⁱ	0.84	2.03	2.832 (5)	159

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

The space group $P2_12_12_1$ was uniquely assigned from the systematic absences. All H atoms were located in difference maps and then treated as riding atoms, with distances C–H = 0.95 Å, N–H = 0.88 Å and O–H = 0.84 Å, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C, N, O})$. In the absence of significant anomalous scattering, the Flack (1983)

parameter was indeterminate (Flack & Bernardinelli, 2000). Accordingly, Friedel equivalent reflections were merged prior to the final refinement. It was therefore not possible to establish the absolute configuration of the molecules in the crystal selected for data collection, but this has no chemical significance.

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *OSCAIL* (McArdle, 2003) and *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *OSCAIL* and *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PRPKAPPA* (Ferguson, 1999).

The X-ray data were collected at the EPSRC X-Ray Crystallographic Service, University of Southampton, England; the authors thank the staff of the Service for all their help and advice. JLW thanks CNPq and FAPERJ for financial support.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: SK1894). Services for accessing these data are described at the back of the journal.

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supporting information

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Computing details

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *OSCAIL* (McArdle, 2003) and *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *OSCAIL* and *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PRPKAPPA* (Ferguson, 1999).

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$C_{11}H_{10}N_4O \cdot H_2O$

$M_r = 232.25$

Orthorhombic, $P2_12_12_1$

Hall symbol: P 2ac 2ab

$a = 6.4224$ (3) Å

$b = 7.2115$ (5) Å

$c = 23.6073$ (16) Å

$V = 1093.38$ (12) Å³

$Z = 4$

$F(000) = 488$

$D_x = 1.411$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 1237 reflections

$\theta = 3.0$ – 26.5°

$\mu = 0.10$ mm⁻¹

$T = 120$ K

Needle, yellow

$0.44 \times 0.06 \times 0.06$ mm

Data collection

Nonius KappaCCD area-detector
diffractometer

Radiation source: Bruker Nonius FR91 rotating
anode

Graphite monochromator

Detector resolution: 9.091 pixels mm⁻¹

φ and ω scans

Absorption correction: multi-scan
(*SADABS*; Sheldrick, 2003)

$T_{\min} = 0.967$, $T_{\max} = 0.994$

5095 measured reflections

1279 independent reflections

1157 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.054$

$\theta_{\max} = 26.5^\circ$, $\theta_{\min} = 3.0^\circ$

$h = -7 \rightarrow 7$

$k = -8 \rightarrow 8$

$l = -17 \rightarrow 29$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.054$

$wR(F^2) = 0.148$

$S = 1.17$

1279 reflections

155 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

$$w = 1/[\sigma^2(F_o^2) + (0.0372P)^2 + 2.0901P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} < 0.001$$

$$\Delta\rho_{\max} = 0.35 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.41 \text{ e } \text{\AA}^{-3}$$

Extinction correction: *SHELXL97* (Sheldrick, 1997), $F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.031 (6)

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.6865 (6)	0.2980 (5)	0.66359 (13)	0.0284 (8)
N11	0.1197 (7)	0.3659 (6)	0.80686 (15)	0.0246 (9)
N17	0.4058 (7)	0.2053 (5)	0.61219 (13)	0.0210 (9)
N21	0.7902 (6)	-0.0358 (5)	0.49180 (14)	0.0204 (9)
N27	0.5395 (6)	0.1447 (5)	0.56955 (14)	0.0195 (8)
C12	0.0430 (8)	0.3915 (6)	0.75496 (18)	0.0225 (10)
C13	0.1532 (7)	0.3589 (6)	0.70543 (17)	0.0186 (10)
C14	0.3577 (7)	0.3029 (6)	0.70943 (17)	0.0159 (9)
C15	0.4432 (8)	0.2752 (6)	0.76360 (17)	0.0239 (11)
C16	0.3173 (9)	0.3077 (7)	0.81000 (18)	0.0281 (12)
C17	0.4967 (7)	0.2699 (6)	0.65957 (17)	0.0188 (9)
C22	0.5847 (7)	-0.0004 (6)	0.48168 (17)	0.0175 (9)
C23	0.5351 (8)	-0.0775 (6)	0.42930 (18)	0.0223 (10)
C24	0.7161 (8)	-0.1591 (6)	0.40792 (18)	0.0229 (11)
C25	0.8724 (8)	-0.1323 (6)	0.44730 (18)	0.0227 (11)
C26	0.4532 (8)	0.0856 (6)	0.52368 (16)	0.0214 (10)
O2	0.9913 (5)	0.0839 (4)	0.59806 (12)	0.0215 (8)
H12	-0.0961	0.4349	0.7517	0.027*
H13	0.0890	0.3749	0.6695	0.022*
H15	0.5832	0.2355	0.7682	0.029*
H16	0.3747	0.2874	0.8466	0.034*
H17	0.2741	0.1722	0.6103	0.025*
H21	0.8591	-0.0017	0.5223	0.024*
H23	0.4027	-0.0750	0.4114	0.029*
H24	0.7293	-0.2218	0.3727	0.030*
H25	1.0123	-0.1737	0.4440	0.030*
H26	0.3076	0.0982	0.5177	0.026*
H2A	0.8869	0.1511	0.6042	0.026*
H2B	0.9824	0.0006	0.6228	0.026*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0255 (19)	0.0358 (19)	0.0238 (16)	0.0008 (18)	0.0024 (16)	-0.0079 (15)
N11	0.027 (2)	0.028 (2)	0.0193 (18)	-0.002 (2)	0.0027 (16)	-0.0031 (16)
N17	0.026 (2)	0.0214 (18)	0.0153 (17)	0.0001 (18)	0.0024 (15)	-0.0037 (15)
N21	0.027 (2)	0.0187 (19)	0.0155 (16)	0.0018 (17)	0.0005 (16)	-0.0006 (15)
N27	0.025 (2)	0.0180 (17)	0.0158 (16)	0.0027 (17)	0.0038 (16)	-0.0022 (14)
C12	0.028 (3)	0.018 (2)	0.022 (2)	0.003 (2)	0.000 (2)	-0.0032 (18)
C13	0.017 (2)	0.022 (2)	0.018 (2)	0.0004 (19)	-0.0024 (18)	-0.0005 (17)

C14	0.014 (2)	0.0151 (19)	0.0182 (19)	0.0006 (18)	0.0014 (17)	-0.0020 (16)
C15	0.029 (3)	0.022 (2)	0.020 (2)	0.001 (2)	-0.002 (2)	-0.0006 (18)
C16	0.037 (3)	0.034 (3)	0.014 (2)	0.003 (3)	-0.001 (2)	0.0036 (19)
C17	0.018 (2)	0.019 (2)	0.019 (2)	0.0025 (19)	-0.0003 (18)	-0.0008 (17)
C22	0.019 (2)	0.017 (2)	0.0168 (19)	0.0012 (19)	0.0001 (18)	0.0005 (16)
C23	0.026 (3)	0.023 (2)	0.018 (2)	-0.004 (2)	-0.001 (2)	-0.0003 (17)
C24	0.033 (3)	0.020 (2)	0.016 (2)	0.000 (2)	0.006 (2)	-0.0024 (18)
C25	0.028 (3)	0.018 (2)	0.022 (2)	0.004 (2)	0.007 (2)	-0.0009 (18)
C26	0.028 (3)	0.021 (2)	0.016 (2)	0.000 (2)	-0.0001 (19)	0.0018 (16)
O2	0.0223 (18)	0.0231 (15)	0.0192 (14)	0.0020 (14)	0.0010 (14)	0.0013 (13)

Geometric parameters (Å, °)

N11—C12	1.333 (6)	C17—O1	1.240 (6)
N11—C16	1.339 (7)	N17—H17	0.88
C12—C13	1.387 (6)	N21—C22	1.365 (6)
C12—H12	0.95	C22—C23	1.393 (6)
C13—C14	1.377 (6)	C23—C24	1.397 (7)
C13—H13	0.95	C24—C25	1.382 (7)
C14—C15	1.406 (6)	C25—N21	1.366 (5)
C14—C17	1.497 (6)	N21—H21	0.88
C17—N17	1.345 (5)	C23—H23	0.95
N17—N27	1.393 (5)	C24—H24	0.95
N27—C26	1.289 (5)	C25—H25	0.95
C26—C22	1.442 (6)	C26—H26	0.95
C15—C16	1.382 (6)	O2—H2A	0.84
C15—H15	0.95	O2—H2B	0.84
C16—H16	0.95		
C12—N11—C16	116.4 (4)	N27—N17—H17	118.0
N11—C12—C13	124.3 (4)	N17—N27—C26	116.5 (4)
N11—C12—H12	117.9	C22—N21—C25	109.5 (4)
C13—C12—H12	117.9	C22—N21—H21	125.2
C14—C13—C12	118.6 (4)	C25—N21—H21	125.2
C14—C13—H13	120.7	N21—C22—C23	107.5 (4)
C12—C13—H13	120.7	N21—C22—C26	121.7 (4)
C13—C14—C15	118.5 (4)	C23—C22—C26	130.4 (4)
C13—C14—C17	124.2 (4)	C22—C23—C24	107.4 (4)
C15—C14—C17	117.4 (4)	C22—C23—H23	126.3
C16—C15—C14	117.9 (4)	C24—C23—H23	126.3
C16—C15—H15	121.0	C25—C24—C23	107.6 (4)
C14—C15—H15	121.0	C25—C24—H24	126.2
N11—C16—C15	124.3 (4)	C23—C24—H24	126.2
N11—C16—H16	117.8	N21—C25—C24	108.0 (4)
C15—C16—H16	117.8	N21—C25—H25	126.0
O1—C17—N17	123.2 (4)	C24—C25—H25	126.0
O1—C17—C14	120.0 (4)	N27—C26—C22	117.9 (4)
C14—C17—N17	116.8 (4)	N27—C26—H26	121.1

C17—N17—N27	116.2 (4)	C22—C26—H26	121.1
C17—N17—H17	123.6	H2A—O2—H2B	103.7
C16—N11—C12—C13	1.1 (7)	C14—C17—N17—N27	-169.2 (4)
N11—C12—C13—C14	-2.5 (7)	C17—N17—N27—C26	-178.9 (4)
C12—C13—C14—C15	2.1 (6)	C25—N21—C22—C23	0.2 (5)
C12—C13—C14—C17	-177.6 (4)	C25—N21—C22—C26	174.5 (4)
C13—C14—C15—C16	-0.6 (6)	N21—C22—C23—C24	-0.4 (5)
C17—C14—C15—C16	179.1 (4)	C26—C22—C23—C24	-174.0 (4)
C12—N11—C16—C15	0.6 (7)	C22—C23—C24—C25	0.4 (5)
C14—C15—C16—N11	-0.8 (7)	C22—N21—C25—C24	0.0 (5)
C13—C14—C17—O1	149.0 (5)	C23—C24—C25—N21	-0.2 (5)
C15—C14—C17—O1	-30.7 (6)	N17—N27—C26—C22	-172.1 (4)
C13—C14—C17—N17	-32.6 (6)	N21—C22—C26—N27	6.4 (6)
C15—C14—C17—N17	147.6 (4)	N27—C26—C22—C23	179.3 (4)
O1—C17—N17—N27	9.1 (6)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O2—H2A...O1	0.84	2.18	2.934 (5)	150
O2—H2A...N27	0.84	2.38	3.011 (5)	133
N21—H21...O2	0.88	2.07	2.950 (5)	174
N17—H17...O2 ⁱ	0.88	1.95	2.822 (5)	173
O2—H2B...N11 ⁱⁱ	0.84	2.03	2.832 (5)	159

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