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A hydrogen-bonded chain of edge-fused rings in 5-nitroisatin

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Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.005 Å
R factor = 0.061
wR factor = 0.109
Data-to-parameter ratio = 14.7

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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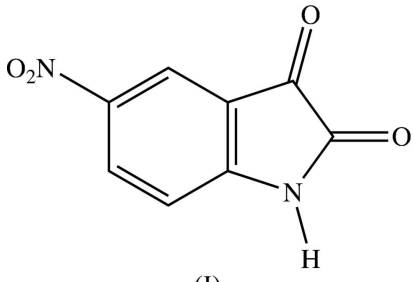
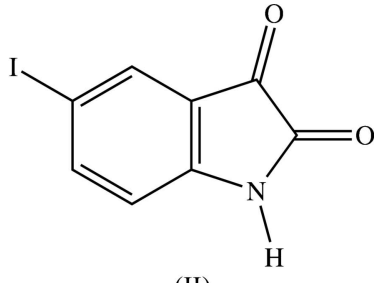
The title compound, $C_8H_4N_2O_4$, crystallizes with $Z' = 2$. The molecules are linked by a combination of N—H···O and C—H···O hydrogen bonds into chains of edge-fused $R_4^4(16)$ and $R_4^4(26)$ rings.

Comment

We report here the molecular and supramolecular structure of 5-nitroisatin (I), whose behaviour is briefly compared with that of 5-iodoisatin (II), which we reported recently (Garden *et al.*, 2006).



(I)



(II)

Compound (I) crystallizes with $Z' = 2$ in the space group $P\overline{1}$ (Fig. 1), and the two molecules have very similar dimensions. Both exhibit long bonds, C11—C12 and C21—C22, between the two carbonyl groups (Table 1), as typically found in isatins (Palenik *et al.*, 1990; Garden *et al.*, 2006), while the dihedral angles between the nitro groups and the adjacent aryl rings are 10.4 (2)° in molecule 1 and 7.4 (2)° in molecule 2.

The molecules are linked into chains of edge-fused rings by a combination of N—H···O and C—H···O hydrogen bonds (Table 2). The N—H···O hydrogen bonds link groups of four molecules, two of each type, into centrosymmetric $R_4^4(16)$ rings (Bernstein *et al.*, 1995) (Fig. 2), and these tetramolecular aggregates are linked by a single C—H···O hydrogen bond into a chain of edge-fused rings along [001], with $R_4^4(16)$ rings centred at $(\frac{1}{2}, \frac{1}{2}, n + \frac{1}{2})$ (n = zero or integer) alternating with $R_4^4(26)$ rings centred at $(\frac{1}{2}, \frac{1}{2}, n)$ (n = zero or integer) (Fig. 3).

These chain of rings are weakly linked by a sheared, parallel (type III, Allen *et al.*, 1998) carbonyl–carbonyl interaction. Atom O11 in the molecule at (x, y, z), which lies in the chain along $(\frac{1}{2}, \frac{1}{2}, z)$, makes a short dipolar contact with atom C22 in the molecule at $(-x, 1 - y, 1 - z)$, which is part of the chain along $(0, \frac{1}{2}, z)$; the key dimensions are O11···C22^{i} = 2.835 (4) Å, O11···O22^{i} = 3.266 (3) Å, C11—O11···C22^{i} = 145.8 (2)° and C11—O11···O22^{i} = 163.9 (2)° [symmetry code: (i) $-x, 1 - y, 1 - z$]. Propagation by inversion of this interaction links the chains into sheets parallel to (010).

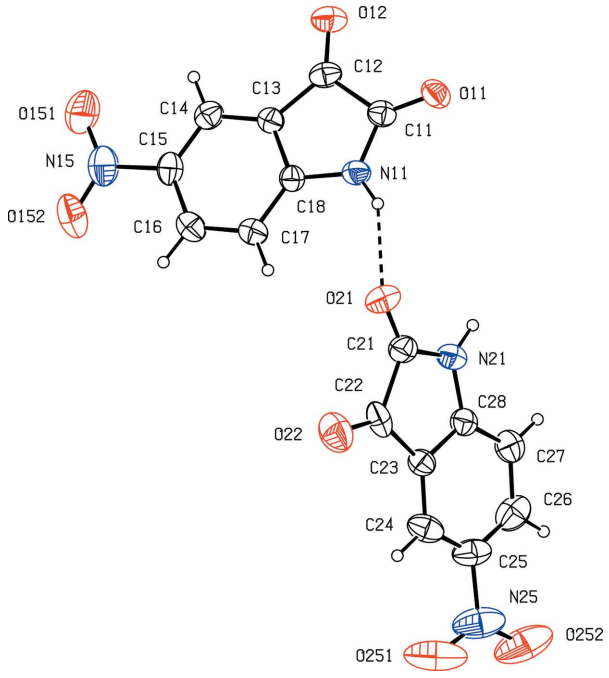


Figure 1
The two independent molecules of compound (I), showing the atom-labelling scheme and the hydrogen-bond (dashed line) within the selected asymmetric unit. Displacement ellipsoids are drawn at the 30% probability level.

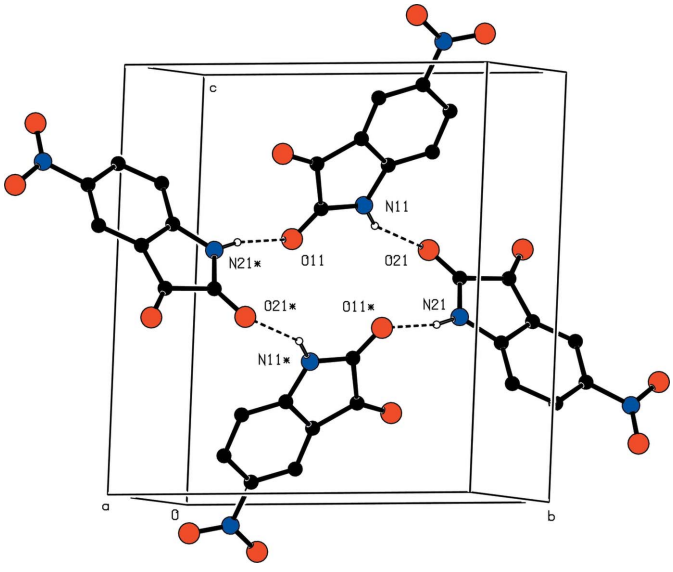


Figure 2
Part of the crystal structure of compound (I), showing the formation of a centrosymmetric tetramolecular aggregate built from N—H···O hydrogen bonds. For the sake of clarity, H atoms bonded to C atoms have been omitted. Atoms marked with an asterisk (*) are at the symmetry position $(1-x, 1-y, 1-z)$, and hydrogen bonds are shown as dashed lines

In 5-iodoisatin, (II), by contrast, which crystallizes with $Z' = 1$, the molecules are linked by a combination of one N—H···O hydrogen bond, one C—H···O hydrogen bond and one iodo–carbonyl interaction into sheets containing alternating

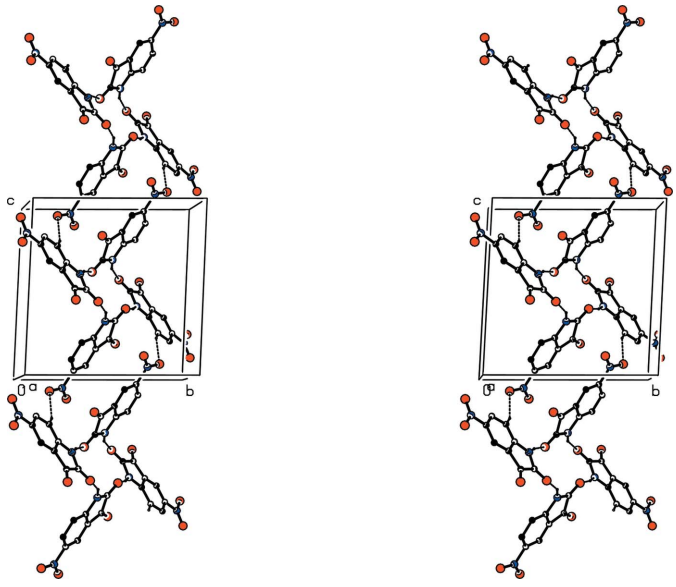


Figure 3
A stereoscopic view of part of the crystal structure of compound (I), showing the formation of a chain of edge-fused $R_4^4(16)$ and $R_4^4(26)$ rings along [001]. Hydrogen bonds are shown as dashed lines, and for the sake of clarity, H atoms not involved in the motifs shown have been omitted.

columns of $R_2^2(9)$ and $R_4^3(16)$ rings, while in isatin itself, the molecules are linked by paired N—H···O hydrogen bonds into $R_2^2(8)$ dimers which are themselves linked into sheets by aromatic π–π stacking interactions (Garden *et al.*, 2006).

Experimental

A commercial sample (Aldrich) of 5-nitroisatin was recrystallized from ethanol.

Crystal data

$C_8H_4N_2O_4$
$M_r = 192.13$
Triclinic, $P\overline{1}$
$a = 5.5595$ (6) Å
$b = 12.0772$ (13) Å
$c = 12.2795$ (14) Å
$\alpha = 87.322$ (3)°
$\beta = 87.355$ (3)°
$\gamma = 83.049$ (3)°
$V = 816.85$ (16) Å^3
$Z = 4$
$D_x = 1.562$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.13$ mm^{-1}
$T = 291$ (2) K
Thick plate, colourless
0.28 × 0.12 × 0.07 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min} = 0.954$, $T_{max} = 0.991$
6130 measured reflections
4096 independent reflections
1331 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$
$\theta_{max} = 28.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.061$
$wR(F^2) = 0.109$
$S = 1.00$
4096 reflections
253 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0209P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.47$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C11—C12	1.558 (4)	C21—C22	1.552 (4)
C14—C15—N15—O151	−11.5 (5)	C24—C25—N25—O251	8.0 (6)
C14—C15—N15—O152	169.8 (3)	C24—C25—N25—O252	−173.5 (4)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N11—H11···O21	0.86	2.11	2.888 (3)	151
N21—H21···O11^{i}	0.86	2.03	2.875 (3)	168
C27—H27···O152^{ii}	0.93	2.43	3.272 (4)	151

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

All H atoms were located in difference maps and then treated as riding atoms, with C—H = 0.93 Å, N—H = 0.86 Å and U_{iso}(H) = $1.2U_{eq}$(C,*N*).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PRPKAPPA* (Ferguson, 1999).

X-ray data were collected at the University of Aberdeen; the authors thank the University of Aberdeen for funding the purchase of the diffractometer. JLW thanks CNPq and FAPERJ for financial support.

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supporting information

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5-nitroisatin

Crystal data

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Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 5.5595$ (6) Å
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$c = 12.2795$ (14) Å
$\alpha = 87.322$ (3)°
$\beta = 87.355$ (3)°
$\gamma = 83.049$ (3)°
$V = 816.85$ (16) Å^3
$Z = 4$
$F(000) = 392$
$D_x = 1.562$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4096 reflections
$\theta = 2.3$–$28.5°$
$\mu = 0.13$ mm^{-1}
$T = 291$ K
Plate, colourless
0.28 × 0.12 × 0.07 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Radiation source: fine-focus sealed X-ray tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2000)
$T_{min} = 0.954$, $T_{max} = 0.991$
6130 measured reflections
4096 independent reflections
1331 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$
$\theta_{max} = 28.5°$, $\theta_{min} = 2.3°$
$h = -7 \rightarrow 7$
$k = -9 \rightarrow 16$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.061$
$wR(F^2) = 0.109$
$S = 1.00$
4096 reflections
253 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
$w = 1/[\sigma^2(F_o^2) + (0.0209P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.47$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
N11	0.3270 (4)	0.52765 (19)	0.6854 (2)	0.0572 (7)
C11	0.5305 (5)	0.4543 (3)	0.6734 (3)	0.0540 (9)

O11	0.5875 (3)	0.39001 (17)	0.60197 (17)	0.0665 (6)
C12	0.6815 (6)	0.4705 (3)	0.7740 (3)	0.0601 (9)
O12	0.8707 (4)	0.41752 (17)	0.79350 (18)	0.0800 (7)
C13	0.5357 (5)	0.5591 (2)	0.8353 (2)	0.0502 (8)
C14	0.5719 (5)	0.6104 (3)	0.9294 (2)	0.0596 (9)
C15	0.3956 (6)	0.6924 (3)	0.9633 (3)	0.0604 (9)
N15	0.4302 (7)	0.7516 (3)	1.0631 (3)	0.0870 (10)
O151	0.5978 (6)	0.7118 (2)	1.1205 (2)	0.1182 (11)
O152	0.2903 (5)	0.8343 (2)	1.0838 (2)	0.1104 (10)
C16	0.1877 (6)	0.7245 (3)	0.9071 (3)	0.0639 (9)
C17	0.1489 (5)	0.6716 (2)	0.8130 (3)	0.0625 (9)
C18	0.3247 (5)	0.5898 (2)	0.7790 (2)	0.0504 (8)
N21	−0.0737 (4)	0.71675 (19)	0.4343 (2)	0.0621 (8)
C21	−0.1946 (6)	0.6865 (3)	0.5280 (3)	0.0621 (9)
O21	−0.1308 (4)	0.61082 (18)	0.59215 (18)	0.0763 (7)
C22	−0.4299 (6)	0.7701 (3)	0.5318 (3)	0.0698 (10)
O22	−0.5799 (5)	0.7723 (2)	0.6023 (2)	0.1049 (9)
C23	−0.4190 (5)	0.8428 (2)	0.4307 (2)	0.0549 (8)
C24	−0.5712 (6)	0.9294 (3)	0.3880 (3)	0.0731 (10)
C25	−0.5048 (7)	0.9777 (3)	0.2914 (4)	0.0791 (11)
N25	−0.6688 (8)	1.0689 (3)	0.2399 (4)	0.1154 (15)
O251	−0.8492 (6)	1.1031 (3)	0.2982 (3)	0.1604 (17)
O252	−0.6190 (6)	1.1048 (3)	0.1501 (3)	0.1631 (17)
C26	−0.2895 (7)	0.9444 (3)	0.2369 (3)	0.0812 (11)
C27	−0.1306 (6)	0.8572 (3)	0.2793 (3)	0.0706 (10)
C28	−0.2009 (5)	0.8062 (2)	0.3768 (3)	0.0557 (8)
H11	0.2117	0.5352	0.6403	0.069*
H14	0.7106	0.5903	0.9688	0.072*
H16	0.0742	0.7815	0.9323	0.077*
H17	0.0088	0.6909	0.7744	0.075*
H21	0.0656	0.6843	0.4129	0.075*
H24	−0.7167	0.9545	0.4243	0.088*
H26	−0.2496	0.9804	0.1711	0.097*
H27	0.0169	0.8341	0.2437	0.085*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N11	0.0482 (17)	0.0578 (17)	0.0646 (19)	0.0037 (13)	−0.0135 (13)	−0.0073 (14)
C11	0.053 (2)	0.046 (2)	0.064 (2)	−0.0084 (16)	−0.0050 (18)	−0.0027 (17)
O11	0.0613 (15)	0.0629 (15)	0.0755 (17)	0.0028 (11)	−0.0079 (12)	−0.0256 (12)
C12	0.048 (2)	0.061 (2)	0.071 (2)	−0.0081 (17)	−0.0072 (18)	0.0146 (18)
O12	0.0617 (15)	0.0758 (16)	0.0988 (19)	0.0089 (12)	−0.0162 (13)	0.0053 (13)
C13	0.050 (2)	0.049 (2)	0.051 (2)	−0.0031 (15)	−0.0012 (17)	−0.0018 (16)
C14	0.053 (2)	0.067 (2)	0.059 (2)	−0.0110 (17)	−0.0023 (18)	0.0049 (18)
C15	0.070 (2)	0.065 (2)	0.051 (2)	−0.0243 (19)	0.0047 (19)	−0.0083 (18)
N15	0.098 (3)	0.092 (3)	0.077 (3)	−0.032 (2)	0.007 (2)	−0.019 (2)
O151	0.131 (3)	0.134 (3)	0.099 (2)	−0.029 (2)	−0.035 (2)	−0.0329 (18)

O152	0.118 (2)	0.116 (2)	0.101 (2)	−0.0201 (18)	0.0192 (18)	−0.0535 (18)
C16	0.065 (2)	0.055 (2)	0.071 (3)	−0.0070 (17)	0.008 (2)	−0.0085 (18)
C17	0.055 (2)	0.062 (2)	0.068 (3)	0.0018 (17)	−0.0009 (18)	−0.0056 (18)
C18	0.050 (2)	0.055 (2)	0.046 (2)	−0.0057 (16)	0.0025 (16)	−0.0014 (16)
N21	0.0507 (17)	0.0605 (18)	0.072 (2)	0.0061 (13)	−0.0037 (15)	−0.0008 (15)
C21	0.057 (2)	0.061 (2)	0.070 (3)	−0.0070 (18)	−0.0160 (19)	−0.0118 (19)
O21	0.0721 (16)	0.0747 (17)	0.0816 (18)	−0.0048 (12)	−0.0245 (13)	0.0130 (13)
C22	0.058 (2)	0.084 (3)	0.070 (3)	−0.0134 (19)	0.0164 (19)	−0.038 (2)
O22	0.115 (2)	0.102 (2)	0.097 (2)	−0.0168 (16)	0.0296 (17)	−0.0162 (15)
C23	0.057 (2)	0.049 (2)	0.058 (2)	−0.0044 (16)	−0.0006 (17)	−0.0028 (17)
C24	0.056 (2)	0.051 (2)	0.112 (3)	−0.0058 (18)	−0.003 (2)	−0.008 (2)
C25	0.075 (3)	0.054 (2)	0.110 (4)	−0.009 (2)	−0.033 (2)	0.009 (2)
N25	0.098 (3)	0.071 (3)	0.180 (5)	−0.027 (2)	−0.047 (3)	0.040 (3)
O251	0.098 (3)	0.097 (3)	0.278 (5)	0.005 (2)	−0.036 (3)	0.057 (3)
O252	0.188 (4)	0.120 (3)	0.188 (4)	−0.049 (2)	−0.085 (3)	0.085 (3)
C26	0.107 (3)	0.066 (3)	0.076 (3)	−0.032 (2)	−0.018 (2)	0.013 (2)
C27	0.068 (2)	0.070 (3)	0.075 (3)	−0.0117 (19)	0.007 (2)	−0.008 (2)
C28	0.055 (2)	0.053 (2)	0.061 (2)	−0.0076 (17)	−0.0075 (18)	−0.0078 (17)

Geometric parameters (Å, º)

N11—C11	1.357 (3)	N21—C21	1.363 (4)
N11—C18	1.401 (3)	N21—C28	1.399 (3)
N11—H11	0.86	N21—H21	0.86
C11—O11	1.205 (3)	C21—O21	1.209 (3)
C11—C12	1.558 (4)	C21—C22	1.552 (4)
C12—O12	1.191 (3)	C22—O22	1.173 (3)
C12—C13	1.476 (4)	C22—C23	1.489 (4)
C13—C14	1.371 (4)	C23—C24	1.363 (4)
C13—C18	1.392 (4)	C23—C28	1.388 (4)
C14—C15	1.371 (4)	C24—C25	1.353 (4)
C14—H14	0.93	C24—H24	0.93
C15—C16	1.380 (4)	C25—C26	1.370 (4)
C15—N15	1.479 (4)	C25—N25	1.479 (4)
N15—O152	1.218 (3)	N25—O252	1.200 (4)
N15—O151	1.232 (3)	N25—O251	1.245 (4)
C16—C17	1.384 (4)	C26—C27	1.388 (4)
C16—H16	0.93	C26—H26	0.93
C17—C18	1.368 (3)	C27—C28	1.383 (4)
C17—H17	0.93	C27—H27	0.93
C11—N11—C18	112.8 (3)	C21—N21—C28	112.6 (3)
C11—N11—H11	123.6	C21—N21—H21	123.7
C18—N11—H11	123.6	C28—N21—H21	123.7
O11—C11—N11	129.0 (3)	O21—C21—N21	127.0 (3)
O11—C11—C12	126.2 (3)	O21—C21—C22	128.7 (3)
N11—C11—C12	104.7 (3)	N21—C21—C22	104.3 (3)
O12—C12—C13	130.5 (3)	O22—C22—C23	129.2 (3)

O12—C12—C11	124.4 (3)	O22—C22—C21	124.8 (4)
C13—C12—C11	105.1 (2)	C23—C22—C21	106.0 (3)
C14—C13—C18	120.0 (3)	C24—C23—C28	120.7 (3)
C14—C13—C12	132.9 (3)	C24—C23—C22	133.6 (3)
C18—C13—C12	107.1 (3)	C28—C23—C22	105.7 (2)
C13—C14—C15	117.4 (3)	C25—C24—C23	118.2 (3)
C13—C14—H14	121.3	C25—C24—H24	120.9
C15—C14—H14	121.3	C23—C24—H24	120.9
C14—C15—C16	123.0 (3)	C24—C25—C26	122.4 (3)
C14—C15—N15	119.1 (3)	C24—C25—N25	120.0 (4)
C16—C15—N15	117.9 (3)	C26—C25—N25	117.5 (4)
O152—N15—O151	124.8 (4)	O252—N25—O251	125.8 (4)
O152—N15—C15	118.4 (4)	O252—N25—C25	119.7 (5)
O151—N15—C15	116.9 (4)	O251—N25—C25	114.4 (5)
C15—C16—C17	119.7 (3)	C25—C26—C27	120.4 (3)
C15—C16—H16	120.2	C25—C26—H26	119.8
C17—C16—H16	120.2	C27—C26—H26	119.8
C18—C17—C16	117.4 (3)	C28—C27—C26	117.2 (3)
C18—C17—H17	121.3	C28—C27—H27	121.4
C16—C17—H17	121.3	C26—C27—H27	121.4
C17—C18—C13	122.5 (3)	C27—C28—C23	121.1 (3)
C17—C18—N11	127.2 (3)	C27—C28—N21	127.5 (3)
C13—C18—N11	110.2 (3)	C23—C28—N21	111.4 (3)

C18—N11—C11—O11	−179.5 (3)	C28—N21—C21—O21	178.2 (3)
C18—N11—C11—C12	0.4 (3)	C28—N21—C21—C22	−1.2 (3)
O11—C11—C12—O12	−2.4 (5)	O21—C21—C22—O22	2.3 (6)
N11—C11—C12—O12	177.6 (3)	N21—C21—C22—O22	−178.4 (3)
O11—C11—C12—C13	179.2 (3)	O21—C21—C22—C23	−178.1 (3)
N11—C11—C12—C13	−0.8 (3)	N21—C21—C22—C23	1.3 (3)
O12—C12—C13—C14	2.4 (6)	O22—C22—C23—C24	−1.2 (7)
C11—C12—C13—C14	−179.4 (3)	C21—C22—C23—C24	179.1 (4)
O12—C12—C13—C18	−177.5 (3)	O22—C22—C23—C28	178.7 (4)
C11—C12—C13—C18	0.8 (3)	C21—C22—C23—C28	−0.9 (4)
C18—C13—C14—C15	−0.9 (4)	C28—C23—C24—C25	0.6 (5)
C12—C13—C14—C15	179.3 (3)	C22—C23—C24—C25	−179.4 (4)
C13—C14—C15—C16	−0.1 (5)	C23—C24—C25—C26	−1.4 (6)
C13—C14—C15—N15	−178.6 (3)	C23—C24—C25—N25	177.6 (3)
C14—C15—N15—O151	−11.5 (5)	C24—C25—N25—O251	8.0 (6)
C14—C15—N15—O152	169.8 (3)	C24—C25—N25—O252	−173.5 (4)
C16—C15—N15—O152	−8.7 (4)	C26—C25—N25—O252	5.5 (6)
C16—C15—N15—O151	169.9 (3)	C26—C25—N25—O251	−172.9 (4)
C14—C15—C16—C17	1.2 (5)	C24—C25—C26—C27	0.8 (6)
N15—C15—C16—C17	179.7 (3)	N25—C25—C26—C27	−178.2 (3)
C15—C16—C17—C18	−1.2 (4)	C25—C26—C27—C28	0.6 (5)
C16—C17—C18—C13	0.2 (4)	C26—C27—C28—C23	−1.4 (5)
C16—C17—C18—N11	−178.3 (3)	C26—C27—C28—N21	179.3 (3)
C14—C13—C18—C17	0.9 (4)	C24—C23—C28—C27	0.8 (5)

C12—C13—C18—C17	−179.3 (3)	C22—C23—C28—C27	−179.1 (3)
C14—C13—C18—N11	179.6 (2)	C24—C23—C28—N21	−179.8 (3)
C12—C13—C18—N11	−0.6 (3)	C22—C23—C28—N21	0.3 (4)
C11—N11—C18—C17	178.7 (3)	C21—N21—C28—C27	180.0 (3)
C11—N11—C18—C13	0.1 (3)	C21—N21—C28—C23	0.6 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N11—H11···O21	0.86	2.11	2.888 (3)	151
N21—H21···O11^{i}	0.86	2.03	2.875 (3)	168
C27—H27···O152^{ii}	0.93	2.43	3.272 (4)	151

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) *x*, *y*, *z*−1.