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N-Acetyl-2-hydroxy-*N*′-[methoxy(1-methylindol-2-yl)methyl]benzohydrazide

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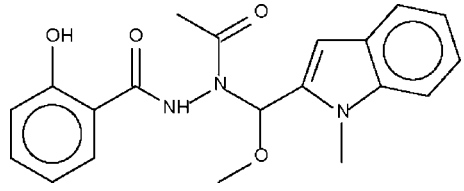
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.047; wR factor = 0.120; data-to-parameter ratio = 16.0.

In the crystal structure of the title Schiff-base, $C_{20}H_{21}N_3O_4$, the amino group forms an N—H···O hydrogen bond to the acetyl group of an adjacent molecule, forming a zigzag chain. The 2-hydroxy group is internally hydrogen bonded to the amido group though an O—H···O hydrogen bond.

Related literature

For medicinal uses of the precursor Schiff base, see: Jin *et al.* (2006); Joshi *et al.* (2008); Szczepankiewicz *et al.* (2001).



Experimental

Crystal data

$C_{20}H_{21}N_3O_4$
M_r = 367.40
Monoclinic, $P2_1/n$
a = 11.0075 (3) Å
b = 10.5197 (3) Å
c = 15.4479 (4) Å
β = 93.967 (2)°
V = 1784.51 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 100 (2) K
0.20 × 0.15 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: none
16316 measured reflections
4072 independent reflections
2646 reflections with $I > 2\sigma(I)$
R_{int} = 0.065

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.120
S = 1.02
4072 reflections
255 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.26 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
O1—H1*o*···O2	0.87 (1)	1.81 (2)	2.599 (2)	150 (3)
N1—H1*n*···O3^{i}	0.85 (1)	2.01 (1)	2.812 (2)	157 (2)

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; 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).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2298).

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supplementary materials

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N-Acetyl-2-hydroxy-*N*'-[methoxy(1-methylindol-2-yl)methyl]benzohydrazide

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Comment

The Schiff base, *N*'-[(1-methyl-1*H*-indol-2-yl)methylene]-2-hydroxybenzohydrazide, exhibits useful medicinal properties (Jin *et al.,* 2006; Joshi *et al.*, 2008; Szczepankiewicz *et al.,* 2001). When dissolved in acetic anhydride, the compound undergoes a reaction to yield the title compound, (I), Fig. 1. Essentially, a mole of methyl acetate has been added across the carbon-nitrogen double-bond. In the crystal structure of (I), the amino group forms an N–H···O hydrogen bond to the acetyl group of an adjacent molecule to result in a zigzag chain that runs along the *b*-axis of the orthorhombic unit cell, Table 1. The 2-hydroxy group is internally hydrogen bonded to the amido group though an O–H···O hydrogen bond, Table 1.

Experimental

2-Hydroxybenzohydrazide was condensed with 1-methylindole-3-carboxaldehyde to yield the corresponding Schiff base. To *N*'-[(1-methyl-1*H*-indol-2-yl)methylene]-2-hydroxybenzohydrazide (0.88 g, 3 mmol) was added acetic anhydride (10 ml). The mixture was heated to 398–403 K until the reactants dissolved completely. After 2 h of heating, the mixture was cooled and then treated with ethyl acetate and saturated aqueous sodium bicarbonate. The organic layer was separated and dried over anhydrous sodium sulfate. The solvent was evaporated and the resulting solid was recrystallized from methanol to give (I) as colorless crystals.

Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.95 to 0.98 Å) and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2–1.5*U*(C). The hydroxy- and ammonium H-atoms were located in a difference Fourier map, and were refined with a distance restraints O–H = N–H = 0.85±0.01 Å; their temperature factors were freely refined.

Figures

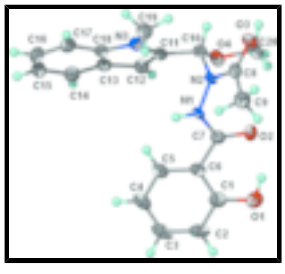


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of (I) drawn at the 70% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

N-Acetyl-2-hydroxy-*N*'-[methoxy(1-methylindol-2- yl)methyl]benzohydrazide

Crystal data

$C_{20}H_{21}N_3O_4$	F_{000} = 776
M_r = 367.40	D_x = 1.367 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 1739 reflections
a = 11.0075 (3) Å	θ = 2.2–21.4º
b = 10.5197 (3) Å	μ = 0.10 mm^{-1}
c = 15.4479 (4) Å	T = 100 (2) K
β = 93.967 (2)º	Block, colorless
V = 1784.51 (8) Å^3	0.20 × 0.15 × 0.10 mm
Z = 4	

Data collection

Bruker SMART APEX diffractometer	2646 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.065
Monochromator: graphite	θ_{max} = 27.5º
T = 100(2) K	θ_{min} = 2.2º
ω scans	h = −14→14
Absorption correction: None	k = −13→13
16316 measured reflections	l = −20→20
4072 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.047	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.120	$w = 1/[\sigma^2(F_o^2) + (0.0466P)^2 + 0.3679P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max}$ = 0.001
4072 reflections	$\Delta\rho_{max}$ = 0.26 e Å^{-3}
255 parameters	$\Delta\rho_{min}$ = −0.26 e Å^{-3}
2 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.75833 (13)	0.62701 (15)	0.28349 (10)	0.0328 (4)
H1O	0.717 (2)	0.5560 (16)	0.2811 (18)	0.069 (10)*
O2	0.57533 (11)	0.47150 (13)	0.28757 (9)	0.0266 (3)
O3	0.27682 (12)	0.25872 (13)	0.22300 (9)	0.0279 (3)
O4	0.41144 (11)	0.35118 (13)	0.43051 (8)	0.0257 (3)
N1	0.38731 (14)	0.55433 (15)	0.29735 (10)	0.0197 (4)
H1N	0.3430 (17)	0.6189 (15)	0.3061 (14)	0.037 (6)*
N2	0.33109 (13)	0.43653 (14)	0.29605 (10)	0.0188 (3)
N3	0.12618 (13)	0.52539 (15)	0.40494 (10)	0.0205 (4)
C1	0.68446 (17)	0.7144 (2)	0.31706 (12)	0.0262 (5)
C2	0.73287 (19)	0.8337 (2)	0.33795 (14)	0.0315 (5)
H2	0.8144	0.8530	0.3262	0.038*
C3	0.6634 (2)	0.9230 (2)	0.37533 (14)	0.0354 (5)
H3	0.6972	1.0042	0.3892	0.042*
C4	0.54370 (19)	0.8971 (2)	0.39356 (13)	0.0308 (5)
H4	0.4966	0.9592	0.4209	0.037*
C5	0.49478 (18)	0.78036 (18)	0.37132 (12)	0.0249 (4)
H5	0.4132	0.7621	0.3837	0.030*
C6	0.56213 (17)	0.68846 (18)	0.33118 (12)	0.0225 (4)
C7	0.51091 (17)	0.56257 (18)	0.30497 (11)	0.0207 (4)
C8	0.31298 (16)	0.36884 (19)	0.22067 (12)	0.0221 (4)
C9	0.33655 (19)	0.4356 (2)	0.13833 (13)	0.0294 (5)
H9A	0.3008	0.3867	0.0889	0.044*
H9B	0.4246	0.4435	0.1337	0.044*
H9C	0.2997	0.5204	0.1383	0.044*
C10	0.30451 (16)	0.38509 (18)	0.38166 (12)	0.0212 (4)
H10	0.2504	0.3091	0.3736	0.025*
C11	0.24263 (16)	0.48432 (18)	0.43178 (12)	0.0208 (4)
C12	0.28551 (17)	0.55066 (18)	0.50327 (12)	0.0227 (4)
H12	0.3624	0.5400	0.5343	0.027*
C13	0.19310 (17)	0.63891 (18)	0.52267 (12)	0.0222 (4)
C14	0.18300 (18)	0.73351 (19)	0.58605 (12)	0.0261 (5)
H14	0.2474	0.7477	0.6291	0.031*
C15	0.07752 (18)	0.8057 (2)	0.58468 (13)	0.0282 (5)
H15	0.0704	0.8708	0.6267	0.034*
C16	−0.01854 (18)	0.7841 (2)	0.52232 (13)	0.0295 (5)
H16	−0.0899	0.8348	0.5230	0.035*
C17	−0.01235 (17)	0.6909 (2)	0.45972 (13)	0.0260 (5)

H17	−0.0785	0.6754	0.4182	0.031*
C18	0.09490 (16)	0.62076 (18)	0.46006 (12)	0.0220 (4)
C19	0.05096 (17)	0.4838 (2)	0.32897 (12)	0.0269 (5)
H19A	−0.0351	0.4872	0.3415	0.040*
H19B	0.0726	0.3963	0.3144	0.040*
H19C	0.0647	0.5397	0.2799	0.040*
C20	0.4677 (2)	0.24041 (19)	0.39780 (14)	0.0313 (5)
H20A	0.5395	0.2183	0.4358	0.047*
H20B	0.4924	0.2574	0.3392	0.047*
H20C	0.4097	0.1696	0.3960	0.047*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0245 (7)	0.0335 (9)	0.0408 (9)	−0.0008 (7)	0.0048 (6)	0.0009 (7)
O2	0.0224 (7)	0.0240 (8)	0.0339 (8)	0.0036 (6)	0.0054 (6)	−0.0027 (6)
O3	0.0311 (8)	0.0184 (8)	0.0342 (8)	−0.0058 (6)	0.0016 (6)	−0.0067 (6)
O4	0.0282 (7)	0.0211 (8)	0.0272 (7)	0.0051 (6)	−0.0028 (6)	−0.0001 (6)
N1	0.0201 (8)	0.0107 (8)	0.0284 (9)	−0.0007 (7)	0.0024 (7)	−0.0012 (7)
N2	0.0219 (8)	0.0112 (8)	0.0235 (8)	−0.0031 (6)	0.0023 (6)	−0.0011 (7)
N3	0.0213 (8)	0.0190 (9)	0.0213 (8)	−0.0025 (7)	0.0010 (6)	−0.0028 (7)
C1	0.0270 (10)	0.0277 (12)	0.0236 (10)	−0.0010 (9)	−0.0011 (8)	0.0057 (9)
C2	0.0291 (11)	0.0302 (12)	0.0345 (12)	−0.0109 (10)	−0.0027 (9)	0.0081 (10)
C3	0.0452 (13)	0.0230 (12)	0.0364 (12)	−0.0101 (10)	−0.0088 (10)	0.0048 (10)
C4	0.0420 (13)	0.0197 (11)	0.0297 (11)	−0.0021 (9)	−0.0028 (10)	−0.0017 (9)
C5	0.0296 (10)	0.0209 (11)	0.0239 (10)	−0.0027 (9)	−0.0014 (8)	0.0013 (9)
C6	0.0252 (10)	0.0184 (10)	0.0236 (10)	−0.0025 (8)	0.0000 (8)	0.0049 (8)
C7	0.0243 (10)	0.0205 (10)	0.0172 (9)	−0.0013 (8)	0.0020 (7)	0.0030 (8)
C8	0.0194 (9)	0.0207 (11)	0.0259 (10)	0.0033 (8)	0.0002 (8)	−0.0026 (8)
C9	0.0338 (11)	0.0306 (12)	0.0241 (10)	−0.0007 (10)	0.0028 (9)	−0.0032 (9)
C10	0.0228 (9)	0.0176 (10)	0.0232 (10)	−0.0010 (8)	0.0007 (8)	0.0005 (8)
C11	0.0222 (9)	0.0175 (10)	0.0228 (9)	−0.0016 (8)	0.0022 (8)	0.0017 (8)
C12	0.0238 (10)	0.0231 (11)	0.0213 (9)	0.0003 (8)	0.0008 (8)	0.0007 (8)
C13	0.0251 (10)	0.0199 (10)	0.0218 (10)	−0.0024 (8)	0.0036 (8)	0.0030 (8)
C14	0.0304 (11)	0.0268 (12)	0.0216 (10)	−0.0033 (9)	0.0043 (8)	−0.0024 (9)
C15	0.0356 (11)	0.0238 (11)	0.0263 (10)	0.0006 (9)	0.0090 (9)	−0.0047 (9)
C16	0.0282 (11)	0.0289 (12)	0.0326 (11)	0.0042 (9)	0.0101 (9)	0.0009 (10)
C17	0.0229 (10)	0.0266 (11)	0.0286 (11)	−0.0011 (8)	0.0036 (8)	0.0012 (9)
C18	0.0236 (9)	0.0193 (10)	0.0236 (10)	−0.0040 (8)	0.0059 (8)	0.0000 (8)
C19	0.0247 (10)	0.0279 (12)	0.0274 (11)	−0.0023 (9)	−0.0028 (8)	−0.0050 (9)
C20	0.0367 (12)	0.0185 (11)	0.0378 (12)	0.0085 (9)	−0.0026 (10)	0.0007 (9)

Geometric parameters (Å, °)

O1—C1	1.354 (2)	C8—C9	1.491 (3)
O1—H1O	0.871 (10)	C9—H9A	0.9800
O2—C7	1.233 (2)	C9—H9B	0.9800
O3—C8	1.226 (2)	C9—H9C	0.9800
O4—C10	1.400 (2)	C10—C11	1.492 (3)

O4—C20	1.428 (2)	C10—H10	1.0000
N1—C7	1.360 (2)	C11—C12	1.363 (3)
N1—N2	1.385 (2)	C12—C13	1.424 (3)
N1—H1N	0.852 (9)	C12—H12	0.9500
N2—C8	1.368 (2)	C13—C14	1.406 (3)
N2—C10	1.477 (2)	C13—C18	1.413 (3)
N3—C18	1.375 (2)	C14—C15	1.387 (3)
N3—C11	1.389 (2)	C14—H14	0.9500
N3—C19	1.456 (2)	C15—C16	1.399 (3)
C1—C2	1.393 (3)	C15—H15	0.9500
C1—C6	1.406 (3)	C16—C17	1.382 (3)
C2—C3	1.365 (3)	C16—H16	0.9500
C2—H2	0.9500	C17—C18	1.392 (3)
C3—C4	1.393 (3)	C17—H17	0.9500
C3—H3	0.9500	C19—H19A	0.9800
C4—C5	1.375 (3)	C19—H19B	0.9800
C4—H4	0.9500	C19—H19C	0.9800
C5—C6	1.390 (3)	C20—H20A	0.9800
C5—H5	0.9500	C20—H20B	0.9800
C6—C7	1.485 (3)	C20—H20C	0.9800
C1—O1—H1O	106.0 (19)	O4—C10—C11	107.19 (14)
C10—O4—C20	112.71 (14)	N2—C10—C11	109.52 (15)
C7—N1—N2	120.11 (16)	O4—C10—H10	109.6
C7—N1—H1N	121.0 (15)	N2—C10—H10	109.6
N2—N1—H1N	117.1 (15)	C11—C10—H10	109.6
C8—N2—N1	121.13 (15)	C12—C11—N3	110.09 (17)
C8—N2—C10	123.05 (15)	C12—C11—C10	129.33 (17)
N1—N2—C10	115.52 (14)	N3—C11—C10	120.52 (16)
C18—N3—C11	107.92 (15)	C11—C12—C13	106.97 (16)
C18—N3—C19	124.45 (16)	C11—C12—H12	126.5
C11—N3—C19	127.50 (16)	C13—C12—H12	126.5
O1—C1—C2	118.06 (18)	C14—C13—C18	118.61 (18)
O1—C1—C6	122.32 (18)	C14—C13—C12	134.43 (18)
C2—C1—C6	119.6 (2)	C18—C13—C12	106.95 (17)
C3—C2—C1	120.1 (2)	C15—C14—C13	118.93 (18)
C3—C2—H2	119.9	C15—C14—H14	120.5
C1—C2—H2	119.9	C13—C14—H14	120.5
C2—C3—C4	121.1 (2)	C14—C15—C16	120.91 (19)
C2—C3—H3	119.4	C14—C15—H15	119.5
C4—C3—H3	119.4	C16—C15—H15	119.5
C5—C4—C3	118.9 (2)	C17—C16—C15	121.71 (19)
C5—C4—H4	120.5	C17—C16—H16	119.1
C3—C4—H4	120.5	C15—C16—H16	119.1
C4—C5—C6	121.40 (19)	C16—C17—C18	117.16 (18)
C4—C5—H5	119.3	C16—C17—H17	121.4
C6—C5—H5	119.3	C18—C17—H17	121.4
C5—C6—C1	118.71 (18)	N3—C18—C17	129.29 (17)
C5—C6—C7	122.54 (17)	N3—C18—C13	108.07 (16)
C1—C6—C7	118.73 (18)	C17—C18—C13	122.64 (18)

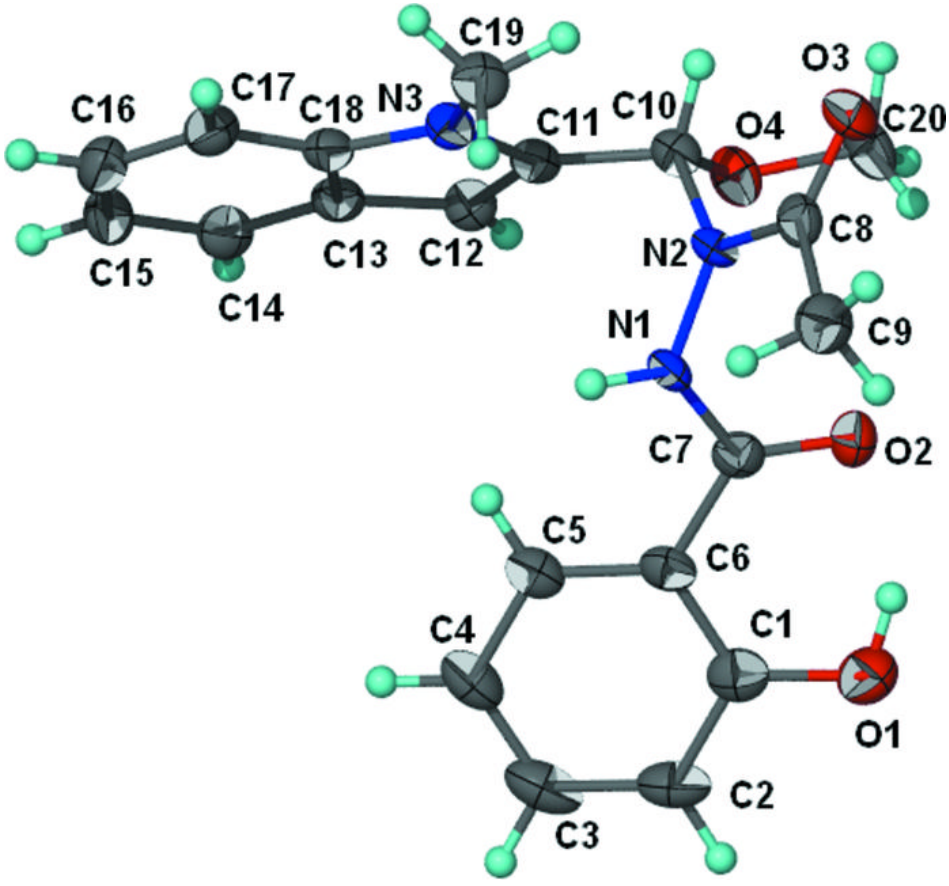
O2—C7—N1	121.25 (17)	N3—C19—H19A	109.5
O2—C7—C6	122.64 (17)	N3—C19—H19B	109.5
N1—C7—C6	116.05 (17)	H19A—C19—H19B	109.5
O3—C8—N2	119.69 (18)	N3—C19—H19C	109.5
O3—C8—C9	123.09 (18)	H19A—C19—H19C	109.5
N2—C8—C9	117.21 (17)	H19B—C19—H19C	109.5
C8—C9—H9A	109.5	O4—C20—H20A	109.5
C8—C9—H9B	109.5	O4—C20—H20B	109.5
H9A—C9—H9B	109.5	H20A—C20—H20B	109.5
C8—C9—H9C	109.5	O4—C20—H20C	109.5
H9A—C9—H9C	109.5	H20A—C20—H20C	109.5
H9B—C9—H9C	109.5	H20B—C20—H20C	109.5
O4—C10—N2	111.40 (15)		
C7—N1—N2—C8	−84.8 (2)	N1—N2—C10—C11	48.99 (19)
C7—N1—N2—C10	89.2 (2)	C18—N3—C11—C12	0.6 (2)
O1—C1—C2—C3	−177.23 (18)	C19—N3—C11—C12	176.65 (18)
C6—C1—C2—C3	2.8 (3)	C18—N3—C11—C10	−176.91 (16)
C1—C2—C3—C4	0.2 (3)	C19—N3—C11—C10	−0.9 (3)
C2—C3—C4—C5	−1.6 (3)	O4—C10—C11—C12	11.2 (3)
C3—C4—C5—C6	−0.1 (3)	N2—C10—C11—C12	−109.8 (2)
C4—C5—C6—C1	3.0 (3)	O4—C10—C11—N3	−171.84 (16)
C4—C5—C6—C7	−178.81 (18)	N2—C10—C11—N3	67.2 (2)
O1—C1—C6—C5	175.68 (17)	N3—C11—C12—C13	−0.6 (2)
C2—C1—C6—C5	−4.3 (3)	C10—C11—C12—C13	176.68 (18)
O1—C1—C6—C7	−2.6 (3)	C11—C12—C13—C14	−178.7 (2)
C2—C1—C6—C7	177.42 (17)	C11—C12—C13—C18	0.3 (2)
N2—N1—C7—O2	19.8 (3)	C18—C13—C14—C15	−0.2 (3)
N2—N1—C7—C6	−162.92 (15)	C12—C13—C14—C15	178.6 (2)
C5—C6—C7—O2	−163.41 (18)	C13—C14—C15—C16	1.0 (3)
C1—C6—C7—O2	14.8 (3)	C14—C15—C16—C17	−0.2 (3)
C5—C6—C7—N1	19.4 (3)	C15—C16—C17—C18	−1.3 (3)
C1—C6—C7—N1	−162.41 (17)	C11—N3—C18—C17	−179.76 (19)
N1—N2—C8—O3	171.07 (16)	C19—N3—C18—C17	4.0 (3)
C10—N2—C8—O3	−2.5 (3)	C11—N3—C18—C13	−0.4 (2)
N1—N2—C8—C9	−10.1 (2)	C19—N3—C18—C13	−176.59 (17)
C10—N2—C8—C9	176.32 (16)	C16—C17—C18—N3	−178.60 (19)
C20—O4—C10—N2	−71.2 (2)	C16—C17—C18—C13	2.1 (3)
C20—O4—C10—C11	168.97 (15)	C14—C13—C18—N3	179.21 (16)
C8—N2—C10—O4	104.46 (19)	C12—C13—C18—N3	0.1 (2)
N1—N2—C10—O4	−69.42 (19)	C14—C13—C18—C17	−1.4 (3)
C8—N2—C10—C11	−137.13 (17)	C12—C13—C18—C17	179.47 (18)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*o*···O2	0.87 (1)	1.81 (2)	2.599 (2)	150 (3)
N1—H1*n*···O3^{i}	0.85 (1)	2.01 (1)	2.812 (2)	157 (2)

Symmetry codes: (i) −*x*+1/2, *y*+1/2, −*z*+1/2.

Fig. 1


C19
C16
C17
C18
N3
C11
C10
O3
O4
C20
C15
C14
C13
C12
N2
C8
N1
C9
C7
O2
C5
C6
C4
C1
O1
C2
C3