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4-[(4-Hydroxy-3-iodo-5-methoxybenzylidene)amino]-1,5-dimethyl-2-phenyl-1*H*-pyrazol-3(2*H*)-one

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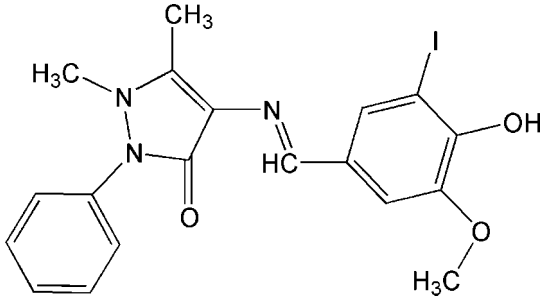
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.008 Å; disorder in main residue; R factor = 0.051; wR factor = 0.088; data-to-parameter ratio = 16.8.

In the title compound, $C_{19}H_{18}IN_3O_3$, intramolecular O—H···O and C—H···O hydrogen bonds stabilize the molecular structure. The 4-hydroxy-3-iodo-5-methoxybenzene group is disordered over two positions, with a site-occupancy ratio of ~9:1. The molecules are linked *via* a weak intermolecular O—H···O hydrogen bond. A short intermolecular I···O contact [3.156 (4) Å] is observed.

Related literature

For general background, see: Belloni *et al.* (2005); Kahwa *et al.* (1986); Parashar *et al.* (1988); Santos *et al.* (2001); Tynan *et al.* (2005).



Experimental

Crystal data

$C_{19}H_{18}IN_3O_3$
M_r = 463.26
Monoclinic, $P2_1/c$
a = 11.855 (3) Å
b = 11.189 (4) Å
c = 13.431 (4) Å
β = 93.089 (5)°
V = 1778.8 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.83 mm^{-1}
T = 113 (2) K
0.04 × 0.04 × 0.02 mm

Data collection

Rigaku Saturn diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.931, T_{max} = 0.964
19273 measured reflections
3493 independent reflections
3195 reflections with $I > 2\sigma(I)$
R_{int} = 0.057

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.088
S = 1.14
3493 reflections
208 parameters
55 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.98 e Å^{-3}
$\Delta\rho_{min}$ = −0.75 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O3^{i}	0.84	1.94	2.668 (5)	144
O1—H1A···O2	0.84	2.24	2.680 (5)	113
O1′—H1′A···O2′	0.84	2.23	2.71 (3)	116
C7—H7A···O3	0.96	2.41	3.112 (6)	130
C7—H7B···O3	0.96	2.43	3.112 (6)	128

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

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *CrystalStructure* (Rigaku/MSC, 2005); software used to prepare material for publication: *CrystalStructure*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2180).

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supplementary materials

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4-[(4-Hydroxy-3-iodo-5-methoxybenzylidene)amino]-1,5-dimethyl-2-phenyl-1*H*-pyrazol-3(2*H*)-one

Z.-L. Jing, S.-Q. Yao, X. Chen and N. Yang

Comment

In order to establish control over the preparation of crystalline solid materials so that their architecture and properties are predictable (Belloni *et al.*, 2005; Tynan *et al.*, 2005; Parashar *et al.*, 1988), the synthesis of new and designed crystal structures has become a major strand of modern chemistry. Metal complexes based on Schiff bases have attracted much attention because they can be utilized as model compounds of active centres in various proteins and enzymes (Kahwa *et al.*, 1986; Santos *et al.*, 2001). As part of an investigation of the coordination properties of Shiff bases functioning as ligands, we report the synthesis and structure of the title compound, (I). In the molecular structure of the title compound (Fig. 1), the expected geometric parameters are observed. The central chomophore (C8—C10/N2/N3) is planar, with an r.m.s. deviation for the fitted atoms of 0.0287 (2) Å. The C8—C10/N2/N3 ring makes dihedral angles of 5.66 (6) and 54.94 (5)° with the benzene C1—C6 and phenyl C13—C18 rings, respectively. The C1—C6 and C13—C18 rings are inclined at an angle of 49.77 (4)°. There are intramolecular O—H···O and C—H···O hydrogen bonds which stabilize the molecular structure. The molecules are linked *via* a weak intermolecular O—H···O hydrogen bond (Fig. 2). A short intermolecular I···O contact is observed [I1···O2(x,-1/2 − y,1/2 + z) 3.156 (4) Å].

Experimental

An anhydrous ethanol solution (50 ml) of 4-hydroxy-3-iodo-5-methoxy- benzaldehyde (2.78 g, 10 mmol) was added to an anhydrous ethanol solution (50 ml) of 4-amino-1,5-dimethyl-2-phenyl-pyrazolidin-3-one (2.03 g, 10 mmol) and the mixture was stirred at 350 K for 6 h under N_2, whereupon a colorless solution appeared. The solvent was removed and the residue recrystallized from anhydrous ethanol. The product was isolated and then dried *in vacuo* to give the title compound in 75% yield. Colorless single crystals suitable for X-ray analysis were obtained by slow evaporation of an anhydrous ethanol solution.

Refinement

The 4-hydroxy-3-iodo-5-methoxybenzene group is disordered over two positions with a site occupancy ratio of 0.907 (2):0.093 (2). In the disordered group, the *C*(phenyl)-O, *C*(methyl)-O and C—I distances were restrained to 1.35 (1), 1.45 (1) and 2.10 (1) Å, respectively, and the C and O atoms of the minor component were refined isotropically. The N-bound H atom was located in a difference Fourier map and its positional parameters were refined, with U_{iso}(H) = 1.2U_{eq}(N). C– and O-bound H atoms were included in calculated positions (C—H = 0.95–0.98 Å and O—H = 0.84 Å), and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C) and 1.5U_{eq}(O).

Figures

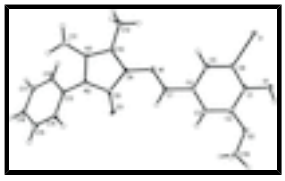

Fig. 1. The molecular structure of (I) with displacement ellipsoids drawn at the 30% probability level. Only the major component of the disordered group is shown.

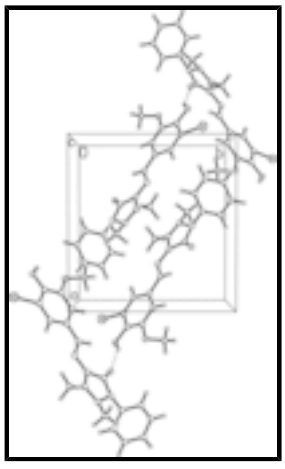

Fig. 2. Packing view of (I) along the *c* axis, showing the intermolecular O—H···O hydrogen bonds (dashed lines).

4-[(4-Hydroxy-3-iodo-5-methoxybenzylidene)amino]-1,5-dimethyl-2-phenyl-1,2- dihydropyrazol-3-one

Crystal data

$C_{19}H_{18}IN_3O_3$	$F(000) = 920$
$M_r = 463.26$	$D_x = 1.730$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71070$ Å
Hall symbol: -P 2ybc	Cell parameters from 4280 reflections
$a = 11.855$ (3) Å	$\theta = 2.5$–$25.0°$
$b = 11.189$ (4) Å	$\mu = 1.83$ mm^{-1}
$c = 13.431$ (4) Å	$T = 113$ K
$\beta = 93.089$ (5)°	Prism, colorless
$V = 1778.8$ (9) Å^3	0.04 × 0.04 × 0.02 mm
$Z = 4$	

Data collection

Rigaku Saturn diffractometer	3493 independent reflections
Radiation source: rotating anode	3195 reflections with $I > 2\sigma(I)$
confocal	$R_{int} = 0.057$
Detector resolution: 7.31 pixels mm^{-1}	$\theta_{max} = 26.0°$, $\theta_{min} = 1.7°$
ω scans	$h = -14 \rightarrow 14$
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)	$k = -13 \rightarrow 13$
$T_{min} = 0.931$, $T_{max} = 0.964$	$l = -16 \rightarrow 16$

19273 measured reflections

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.051$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.088$	H-atom parameters constrained
$S = 1.14$	$w = 1/[\sigma^2(F_o^2) + 9.7939P]$ where $P = (F_o^2 + 2F_c^2)/3$
3493 reflections	$(\Delta/\sigma)_{max} = 0.001$
208 parameters	$\Delta\rho_{max} = 0.98$ e Å^{-3}
55 restraints	$\Delta\rho_{min} = -0.75$ e Å^{-3}

Special details

Experimental. 'College of Sciences Tianjin University of Science and Technology Tianjin 300457 P. *R*. China'

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.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O3	0.3601 (3)	0.2443 (3)	0.8365 (3)	0.0197 (8)	
N1	0.2523 (3)	0.0337 (4)	0.9626 (3)	0.0167 (9)	
N2	0.4805 (3)	0.2506 (4)	0.9779 (3)	0.0165 (9)	
N3	0.5021 (3)	0.1771 (4)	1.0616 (3)	0.0173 (9)	
C7	0.1818 (4)	0.0532 (5)	0.8883 (4)	0.0196 (11)	
H7A	0.1961	0.1180	0.8439	0.023*	0.9097 (17)
H7B	0.1988	0.1100	0.8377	0.023*	0.0903 (17)
C8	0.3450 (4)	0.1096 (5)	0.9814 (4)	0.0166 (11)	
C9	0.3875 (4)	0.2052 (5)	0.9216 (4)	0.0166 (11)	
C10	0.4154 (4)	0.0989 (5)	1.0653 (4)	0.0153 (11)	
C11	0.5658 (5)	0.2262 (5)	1.1479 (4)	0.0270 (13)	
H11A	0.5132	0.2582	1.1951	0.041*	
H11B	0.6152	0.2904	1.1264	0.041*	
H11C	0.6116	0.1630	1.1804	0.041*	
C12	0.4035 (5)	0.0206 (5)	1.1534 (4)	0.0222 (12)	
H12A	0.4688	−0.0329	1.1609	0.033*	

H12B	0.3342	−0.0268	1.1442	0.033*	
H12C	0.3996	0.0701	1.2134	0.033*	
C13	0.5705 (4)	0.3159 (5)	0.9367 (4)	0.0174 (11)	
C14	0.5485 (5)	0.4292 (5)	0.8989 (4)	0.0193 (12)	
H14	0.4751	0.4628	0.9016	0.023*	
C15	0.6341 (5)	0.4932 (5)	0.8572 (4)	0.0252 (13)	
H15	0.6194	0.5707	0.8306	0.030*	
C16	0.7407 (5)	0.4442 (5)	0.8543 (4)	0.0269 (13)	
H16	0.7996	0.4887	0.8265	0.032*	
C17	0.7623 (4)	0.3304 (6)	0.8916 (4)	0.0269 (13)	
H17	0.8356	0.2969	0.8881	0.032*	
C18	0.6779 (4)	0.2654 (5)	0.9339 (4)	0.0213 (12)	
H18	0.6928	0.1879	0.9604	0.026*	
I1	−0.08416 (7)	−0.32209 (4)	1.01007 (4)	0.02000 (14)	0.9097 (17)
O1	−0.2061 (3)	−0.2308 (3)	0.8143 (3)	0.0173 (9)*	0.9097 (17)
H1A	−0.2391	−0.2116	0.7598	0.026*	0.9097 (17)
C1	−0.1153 (2)	−0.1571 (2)	0.8334 (2)	0.0155 (11)*	0.9097 (17)
C2	−0.0926 (2)	−0.0621 (3)	0.7709 (2)	0.0169 (12)*	0.9097 (17)
C3	0.0039 (3)	0.0066 (3)	0.7893 (2)	0.0164 (13)*	0.9097 (17)
H3A	0.0194	0.0716	0.7466	0.020*	0.9097 (17)
C4	0.0778 (3)	−0.0197 (3)	0.8702 (3)	0.0172 (11)*	0.9097 (17)
C5	0.0552 (2)	−0.1147 (3)	0.9327 (2)	0.0165 (13)*	0.9097 (17)
H5A	0.1057	−0.1327	0.9880	0.020*	0.9097 (17)
C6	−0.0414 (2)	−0.1834 (2)	0.9143 (2)	0.0146 (11)*	0.9097 (17)
O2	−0.1732 (3)	−0.0422 (3)	0.6963 (3)	0.0190 (9)*	0.9097 (17)
C19	−0.1766 (9)	0.0740 (8)	0.6520 (8)	0.030 (4)*	0.9097 (17)
H19A	−0.2414	0.0792	0.6036	0.044*	0.9097 (17)
H19B	−0.1067	0.0880	0.6180	0.044*	0.9097 (17)
H19C	−0.1842	0.1345	0.7040	0.044*	0.9097 (17)
I1'	−0.2005 (5)	0.0428 (6)	0.6609 (4)	0.0256 (15)	0.0903 (17)
O2'	−0.043 (2)	−0.3101 (18)	0.918 (2)	0.037 (12)*	0.0903 (17)
O1'	−0.1947 (19)	−0.222 (2)	0.779 (2)	0.0173 (9)*	0.0903 (17)
H1'A	−0.1879	−0.2894	0.8065	0.026*	0.0903 (17)
C1'	−0.1059 (11)	−0.1526 (13)	0.8080 (12)	0.0155 (11)*	0.0903 (17)
C2'	−0.0291 (13)	−0.1998 (16)	0.8793 (15)	0.0169 (12)*	0.0903 (17)
C3'	0.0643 (15)	−0.133 (2)	0.913 (2)	0.0164 (13)*	0.0903 (17)
H3'A	0.1168	−0.1653	0.9617	0.020*	0.0903 (17)
C4'	0.0809 (19)	−0.019 (3)	0.875 (3)	0.0172 (11)*	0.0903 (17)
C5'	0.0041 (17)	0.0280 (19)	0.804 (2)	0.0165 (13)*	0.0903 (17)
H5'A	0.0154	0.1059	0.7778	0.020*	0.0903 (17)
C6'	−0.0893 (10)	−0.0387 (14)	0.7701 (11)	0.0146 (11)*	0.0903 (17)
C19'	−0.097 (15)	−0.321 (5)	1.009 (8)	0.037 (12)*	0.0903 (17)
H19D	−0.1755	−0.3481	0.9947	0.055*	0.0903 (17)
H19E	−0.0977	−0.2438	1.0425	0.055*	0.0903 (17)
H19F	−0.0572	−0.3800	1.0515	0.055*	0.0903 (17)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O3	0.0155 (18)	0.028 (2)	0.0146 (18)	−0.0006 (16)	−0.0044 (14)	0.0050 (16)
N1	0.012 (2)	0.021 (2)	0.016 (2)	−0.0003 (18)	−0.0015 (17)	0.0000 (18)
N2	0.016 (2)	0.020 (2)	0.014 (2)	−0.0026 (18)	−0.0028 (17)	0.0041 (18)
N3	0.018 (2)	0.022 (2)	0.011 (2)	−0.0009 (19)	−0.0049 (17)	0.0019 (19)
C7	0.018 (3)	0.019 (3)	0.022 (3)	−0.001 (2)	0.003 (2)	0.000 (2)
C8	0.014 (3)	0.019 (3)	0.016 (3)	0.001 (2)	0.001 (2)	0.001 (2)
C9	0.012 (2)	0.021 (3)	0.016 (3)	0.000 (2)	0.000 (2)	−0.003 (2)
C10	0.016 (3)	0.015 (3)	0.015 (3)	−0.002 (2)	0.002 (2)	−0.001 (2)
C11	0.028 (3)	0.032 (3)	0.020 (3)	−0.008 (3)	−0.011 (2)	0.004 (2)
C12	0.024 (3)	0.026 (3)	0.017 (3)	−0.003 (2)	−0.001 (2)	0.004 (2)
C13	0.017 (3)	0.022 (3)	0.013 (2)	−0.006 (2)	−0.001 (2)	−0.001 (2)
C14	0.024 (3)	0.018 (3)	0.016 (3)	0.000 (2)	−0.004 (2)	−0.004 (2)
C15	0.037 (3)	0.019 (3)	0.019 (3)	−0.008 (2)	−0.001 (2)	0.002 (2)
C16	0.026 (3)	0.036 (4)	0.018 (3)	−0.016 (3)	0.000 (2)	−0.003 (3)
C17	0.015 (3)	0.043 (4)	0.022 (3)	−0.004 (3)	−0.005 (2)	−0.004 (3)
C18	0.021 (3)	0.016 (3)	0.025 (3)	0.000 (2)	−0.009 (2)	−0.001 (2)
I1	0.0190 (3)	0.0176 (2)	0.0228 (2)	−0.00328 (17)	−0.00413 (16)	0.00546 (17)
I1'	0.015 (3)	0.033 (3)	0.028 (3)	0.003 (3)	−0.006 (2)	0.001 (2)

Geometric parameters (Å, °)

O3—C9	1.251 (6)	I1—C6	2.095 (3)
N1—C7	1.286 (7)	O1—C1	1.369 (4)
N1—C8	1.400 (6)	O1—H1A	0.8400
N2—C9	1.398 (6)	C1—C2	1.3900
N2—N3	1.405 (6)	C1—C6	1.3900
N2—C13	1.428 (6)	C2—O2	1.365 (4)
N3—C10	1.354 (6)	C2—C3	1.3900
N3—C11	1.456 (6)	C3—C4	1.3900
C7—C4'	1.448 (11)	C3—H3A	0.9500
C7—C4	1.487 (6)	C4—C5	1.3900
C7—H7A	0.9599	C5—C6	1.3900
C7—H7B	0.9599	C5—H5A	0.9500
C8—C10	1.371 (7)	O2—C19	1.430 (8)
C8—C9	1.445 (7)	C19—H19A	0.9800
C10—C12	1.485 (7)	C19—H19B	0.9800
C11—H11A	0.9800	C19—H19C	0.9800
C11—H11B	0.9800	I1'—C6'	2.125 (13)
C11—H11C	0.9800	O2'—C2'	1.350 (9)
C12—H12A	0.9800	O2'—C19'	1.421 (11)
C12—H12B	0.9800	O1'—C1'	1.351 (9)
C12—H12C	0.9800	O1'—H1'A	0.8400
C13—C14	1.385 (7)	C1'—C2'	1.3900
C13—C18	1.396 (7)	C1'—C6'	1.3900
C14—C15	1.385 (8)	C2'—C3'	1.3900

C14—H14	0.9500	C3'—C4'	1.3900
C15—C16	1.380 (8)	C3'—H3'A	0.9500
C15—H15	0.9500	C4'—C5'	1.3900
C16—C17	1.387 (9)	C5'—C6'	1.3900
C16—H16	0.9500	C5'—H5'A	0.9500
C17—C18	1.383 (8)	C19'—H19D	0.9800
C17—H17	0.9500	C19'—H19E	0.9800
C18—H18	0.9500	C19'—H19F	0.9800
C7—N1—C8	120.5 (5)	C17—C18—C13	118.6 (5)
C9—N2—N3	108.9 (4)	C17—C18—H18	120.7
C9—N2—C13	124.1 (4)	C13—C18—H18	120.7
N3—N2—C13	120.1 (4)	C1—O1—H1A	109.5
C10—N3—N2	107.6 (4)	O1—C1—C2	121.5 (3)
C10—N3—C11	125.2 (4)	O1—C1—C6	118.4 (3)
N2—N3—C11	118.7 (4)	C2—C1—C6	120.0
N1—C7—C4'	119.9 (10)	O2—C2—C3	125.3 (3)
N1—C7—C4	122.1 (5)	O2—C2—C1	114.7 (3)
N1—C7—H7A	118.8	C3—C2—C1	120.0
C4—C7—H7A	119.0	C4—C3—C2	120.0
N1—C7—H7B	120.7	C4—C3—H3A	120.0
C4'—C7—H7B	119.1	C2—C3—H3A	120.0
C10—C8—N1	122.1 (5)	C3—C4—C5	120.0
C10—C8—C9	107.8 (4)	C3—C4—C7	119.6 (3)
N1—C8—C9	130.0 (5)	C5—C4—C7	120.4 (3)
O3—C9—N2	121.7 (5)	C6—C5—C4	120.0
O3—C9—C8	133.3 (5)	C6—C5—H5A	120.0
N2—C9—C8	104.9 (4)	C4—C5—H5A	120.0
N3—C10—C8	110.1 (4)	C5—C6—C1	120.0
N3—C10—C12	121.0 (4)	C5—C6—I1	121.67 (17)
C8—C10—C12	128.8 (5)	C1—C6—I1	118.26 (17)
N3—C11—H11A	109.5	C2—O2—C19	117.2 (5)
N3—C11—H11B	109.5	C2'—O2'—C19'	119 (2)
H11A—C11—H11B	109.5	C1'—O1'—H1'A	109.5
N3—C11—H11C	109.5	O1'—C1'—C2'	116.9 (9)
H11A—C11—H11C	109.5	O1'—C1'—C6'	123.1 (9)
H11B—C11—H11C	109.5	C2'—C1'—C6'	120.0
C10—C12—H12A	109.5	O2'—C2'—C1'	121.5 (9)
C10—C12—H12B	109.5	O2'—C2'—C3'	118.5 (9)
H12A—C12—H12B	109.5	C1'—C2'—C3'	120.0
C10—C12—H12C	109.5	C4'—C3'—C2'	120.0
H12A—C12—H12C	109.5	C4'—C3'—H3'A	120.0
H12B—C12—H12C	109.5	C2'—C3'—H3'A	120.0
C14—C13—C18	121.0 (5)	C3'—C4'—C5'	120.0
C14—C13—N2	118.7 (5)	C3'—C4'—C7	126.9 (12)
C18—C13—N2	120.3 (5)	C5'—C4'—C7	112.2 (11)
C15—C14—C13	119.6 (5)	C6'—C5'—C4'	120.0
C15—C14—H14	120.2	C6'—C5'—H5'A	120.0
C13—C14—H14	120.2	C4'—C5'—H5'A	120.0
C16—C15—C14	119.8 (5)	C5'—C6'—C1'	120.0

C16—C15—H15	120.1	C5'—C6'—I1'	116.6 (7)
C14—C15—H15	120.1	C1'—C6'—I1'	123.5 (7)
C15—C16—C17	120.4 (5)	O2'—C19'—H19D	109.5
C15—C16—H16	119.8	O2'—C19'—H19E	109.5
C17—C16—H16	119.8	H19D—C19'—H19E	109.5
C18—C17—C16	120.5 (5)	O2'—C19'—H19F	109.5
C18—C17—H17	119.7	H19D—C19'—H19F	109.5
C16—C17—H17	119.7	H19E—C19'—H19F	109.5
C9—N2—N3—C10	−8.7 (5)	O2—C2—C3—C4	177.4 (3)
C13—N2—N3—C10	−160.6 (4)	C1—C2—C3—C4	0.0
C9—N2—N3—C11	−158.3 (5)	C2—C3—C4—C5	0.0
C13—N2—N3—C11	49.7 (7)	C2—C3—C4—C7	179.1 (4)
C8—N1—C7—C4'	−174 (2)	N1—C7—C4—C3	179.2 (4)
C8—N1—C7—C4	−175.3 (4)	C4'—C7—C4—C3	157 (40)
C7—N1—C8—C10	173.3 (5)	N1—C7—C4—C5	−1.8 (6)
C7—N1—C8—C9	−9.1 (8)	C4'—C7—C4—C5	−24 (40)
N3—N2—C9—O3	−170.1 (5)	C3—C4—C5—C6	0.0
C13—N2—C9—O3	−19.4 (8)	C7—C4—C5—C6	−179.1 (4)
N3—N2—C9—C8	6.9 (5)	C4—C5—C6—C1	0.0
C13—N2—C9—C8	157.6 (5)	C4—C5—C6—I1	−176.81 (16)
C10—C8—C9—O3	173.6 (6)	O1—C1—C6—C5	176.4 (2)
N1—C8—C9—O3	−4.3 (10)	C2—C1—C6—C5	0.0
C10—C8—C9—N2	−2.8 (6)	O1—C1—C6—I1	−6.7 (2)
N1—C8—C9—N2	179.3 (5)	C2—C1—C6—I1	176.92 (16)
N2—N3—C10—C8	6.8 (6)	C3—C2—O2—C19	−18.6 (6)
C11—N3—C10—C8	154.0 (5)	C1—C2—O2—C19	159.0 (5)
N2—N3—C10—C12	−170.6 (5)	C19'—O2'—C2'—C1'	−95 (9)
C11—N3—C10—C12	−23.4 (8)	C19'—O2'—C2'—C3'	85 (9)
N1—C8—C10—N3	175.6 (4)	O1'—C1'—C2'—O2'	0.0 (5)
C9—C8—C10—N3	−2.5 (6)	C6'—C1'—C2'—O2'	−180.0 (3)
N1—C8—C10—C12	−7.2 (9)	O1'—C1'—C2'—C3'	−180.0 (3)
C9—C8—C10—C12	174.7 (5)	C6'—C1'—C2'—C3'	0.0
C9—N2—C13—C14	68.8 (7)	O2'—C2'—C3'—C4'	180.0 (3)
N3—N2—C13—C14	−143.6 (5)	C1'—C2'—C3'—C4'	0.0
C9—N2—C13—C18	−110.4 (6)	C2'—C3'—C4'—C5'	0.0
N3—N2—C13—C18	37.2 (7)	C2'—C3'—C4'—C7	−168 (3)
C18—C13—C14—C15	0.3 (8)	N1—C7—C4'—C3'	−23 (3)
N2—C13—C14—C15	−178.9 (5)	C4—C7—C4'—C3'	136 (42)
C13—C14—C15—C16	−0.5 (8)	N1—C7—C4'—C5'	168.3 (5)
C14—C15—C16—C17	0.9 (8)	C4—C7—C4'—C5'	−33 (39)
C15—C16—C17—C18	−1.2 (8)	C3'—C4'—C5'—C6'	0.0
C16—C17—C18—C13	0.9 (8)	C7—C4'—C5'—C6'	170 (3)
C14—C13—C18—C17	−0.5 (8)	C4'—C5'—C6'—C1'	0.0
N2—C13—C18—C17	178.7 (5)	C4'—C5'—C6'—I1'	−179.9 (2)
O1—C1—C2—O2	6.1 (3)	O1'—C1'—C6'—C5'	180.0 (3)
C6—C1—C2—O2	−177.7 (2)	C2'—C1'—C6'—C5'	0.0
O1—C1—C2—C3	−176.2 (2)	O1'—C1'—C6'—I1'	−0.1 (4)
C6—C1—C2—C3	0.0	C2'—C1'—C6'—I1'	179.9 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1A···O3^{i}	0.84	1.94	2.668 (5)	144
O1—H1A···O2	0.84	2.24	2.680 (5)	113
O1'—H1'A···O2'	0.84	2.23	2.71 (3)	116
C7—H7A···O3	0.96	2.41	3.112 (6)	130
C7—H7B···O3	0.96	2.43	3.112 (6)	128

Symmetry codes: (i) −*x*, *y*−1/2, −*z*+3/2.

Fig. 1

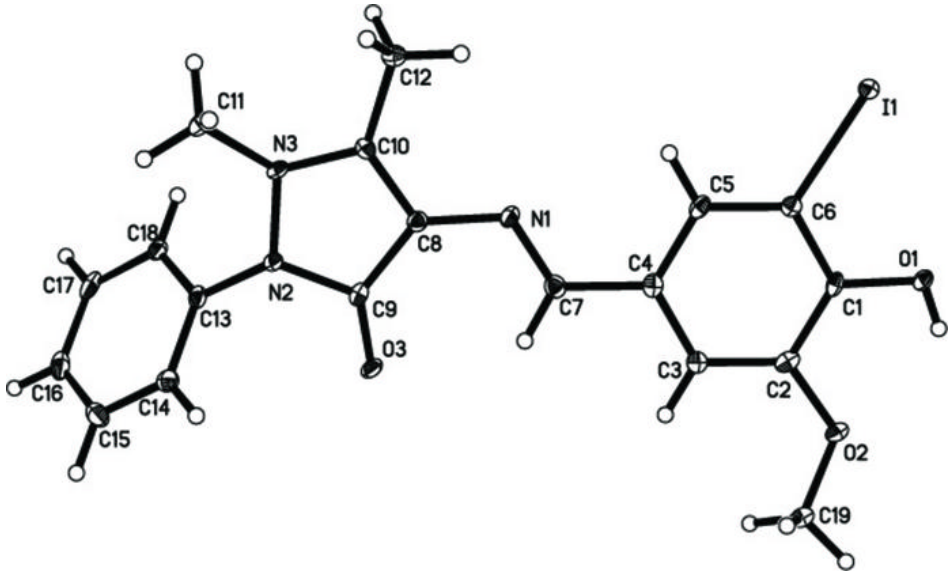
C12
C11
I1
N3
C10
C5
C6
N1
C18
C8
C4
O1
C17
N2
C9
C7
C1
C13
O3
C3
C2
C16
C14
O2
C15
C19

Fig. 2