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(*E*)-*N*′-(4-Hydroxybenzylidene)-4-(quinolin-8-yloxy)butanohydrazide hemihydrate

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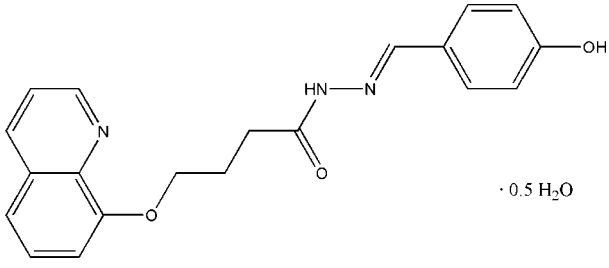
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.005 Å; some non-H atoms missing; R factor = 0.061; wR factor = 0.187; data-to-parameter ratio = 12.9.

In the title compound, $C_{20}H_{19}N_3O_3\cdot0.5H_2O$, the mean planes of the benzene ring and quinoline group make a dihedral angle of 98.6 (3)°. The molecules are connected *via* intermolecular N—H···O and O—H···N hydrogen bonds into infinite chains. The chains are linked by the water molecule through O—H···O hydrogen bonds (the water molecules are located on crystallographic twofold rotation axes).

Related literature

For related literature, see: Allen *et al.* (1987); Chen & Shi (1998); Mona & Wageih (2002).



Experimental

Crystal data

$C_{20}H_{19}N_3O_3\cdot0.5H_2O$
M_r = 358.39
Monoclinic, $C2/c$
a = 29.905 (3) Å
b = 10.4609 (9) Å
c = 11.4613 (10) Å
β = 99.507 (4)°
V = 3536.2 (6) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 295 K
0.28 × 0.26 × 0.23 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.974, T_{max} = 0.979
15979 measured reflections
3117 independent reflections
1697 reflections with $I > 2\sigma(I)$
R_{int} = 0.094

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.187
S = 1.00
3117 reflections
242 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N3^{i}	0.82	1.96	2.766 (4)	168
O4—H20···O2^{ii}	0.85	2.26	3.054 (5)	156
N2—H2···O2^{iii}	0.86	2.09	2.891 (4)	155

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2018).

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supplementary materials

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(*E*)-*N*'-(4-Hydroxybenzylidene)-4-(quinolin-8-yloxy)butanohydrazide hemihydrate

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Comment

8-Hydroxyquinoline and its derivatives constitute well known ligands in coordination chemistry (Chen & Shi, 1998; Mona & Wageih, 2002). In our search for new extractants of metal ions and biologically active materials, the title compound, (I), has been synthesized. We report here its crystal structure. The bond lengths and angles in (I) fall within their expected ranges (Allen *et al.*, 1987). The conformation along the C7—N1—N2—C8—C9—C10—C11—O3 bond sequence is *trans*-(-)*gauche*-*trans*-*trans*-(+)*gauche* (Fig.1). The mean planes of the benzene ring and quinoline group make a dihedral angle of 98.6 (3)°. In the crystal structure (Table and Fig. 2), intermolecular N—H···O and O—H···N hydrogen bonds into infinite chains. The chains was linked by the water molecular through O—H···O hydrogen bonds (H_2O molecules located on 2 axes).

Experimental

4–(Quinolin–8–yl–oxy)butanohydrazide (0.01 mol), 4–hydroxybenzaldehyde (0.01 mol), ethanol (60 ml) and some drops of acetic acid were added to a 100 ml flask and refluxed for 6 h. After cooling to room temperature, the solid product was separated by filtration. Colourless single crystals suitable for *X*–ray diffraction study were obtained by slow evaporation of a *N*,*N*-dimethylformamide solution over a period of two weeks (m.p. 521 K). Calculated for $C_{40}H_{40}N_6O_7$: C 67.02, H 5.63, N 11.72%; found: C 66.98, H 5.58, N 11.77%.

Refinement

All H atoms were placed in idealized positions (C—H = 0.93–0.97 Å, O—H = 0.82–0.85 Å, N—H = 0.86 Å) and refined as riding atoms. For those bound to C, U_{iso}(H) = 1.2U_{eq}(C,*N*) or 1.5U_{eq}(O).

Figures

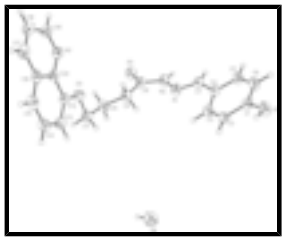

Fig. 1. The molecular structure of (I) with the atoms numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen atoms are drawn as spheres with arbitrary radius.

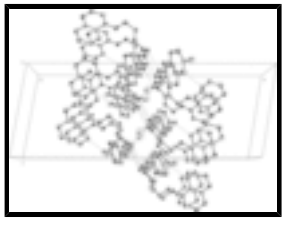

Fig. 2. Detail of (I) showing part of a hydrogen–bonded chain. H atoms and hydrate have been omitted for clarity and the dashed lines represent the O···N contacts of the hydrogen bonds.

(*E*)-*N*′-(4-Hydroxybenzylidene)-4-(quinolin-8-yloxy)butanohydrazide hemihydrate

Crystal data

$C_{20}H_{19}N_3O_3 \cdot 0.5H_2O$	$F_{000} = 1512$
$M_r = 358.39$	$D_x = 1.346$ Mg m^{-3} $D_m = 1.346$ Mg m^{-3} D_m measured by not measured
Monoclinic, $C2/c$	Melting point: 521 K
Hall symbol: -C 2yc	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 29.905$ (3) Å	Cell parameters from 1208 reflections
$b = 10.4609$ (9) Å	$\theta = 2.1$–18.7º
$c = 11.4613$ (10) Å	$\mu = 0.09$ mm^{-1}
$\beta = 99.507$ (4)º	$T = 295$ K
$V = 3536.2$ (6) Å^3	Block, colorless
$Z = 8$	0.28 × 0.26 × 0.23 mm

Data collection

Bruker SMART CCD area-detector diffractometer	3117 independent reflections
Radiation source: fine–focus sealed tube	1697 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.094$
$T = 295$ K	$\theta_{max} = 25.0$º
φ and ω scans	$\theta_{min} = 2.1$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -34 \rightarrow 35$
$T_{min} = 0.974$, $T_{max} = 0.979$	$k = -12 \rightarrow 12$
15979 measured reflections	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.061$	$w = 1/[\sigma^2(F_o^2) + (0.0571P)^2 + 2.4946P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.187$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.00$	$\Delta\rho_{max} = 0.18$ e Å^{-3}
3117 reflections	$\Delta\rho_{min} = -0.36$ e Å^{-3}
242 parameters	Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0039 (7)
Secondary atom site location: difference Fourier map	

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.

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 $F^2 > 2\mathrm{sigma}(F^2)$ 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}
O1	0.35956 (9)	0.2042 (2)	0.9194 (2)	0.0699 (8)
H1	0.3372	0.2085	0.8673	0.105*
O2	0.47282 (8)	1.0823 (2)	0.8757 (2)	0.0676 (8)
O3	0.33289 (8)	1.1129 (2)	0.6432 (2)	0.0605 (7)
O4	0.5000	0.6796 (5)	0.2500	0.1224 (17)
H20	0.4899	0.7286	0.2989	0.184*
N1	0.44358 (9)	0.7579 (3)	0.8779 (3)	0.0567 (8)
N2	0.46700 (9)	0.8721 (3)	0.9037 (3)	0.0572 (8)
H2	0.4907	0.8734	0.9577	0.069*
N3	0.27664 (9)	1.2141 (3)	0.7713 (3)	0.0552 (8)
C1	0.38355 (12)	0.3144 (3)	0.9218 (3)	0.0546 (9)
C2	0.38057 (12)	0.3950 (3)	0.8245 (3)	0.0553 (9)
H2A	0.3622	0.3729	0.7538	0.066*
C3	0.40460 (11)	0.5066 (3)	0.8322 (3)	0.0551 (9)
H3	0.4027	0.5590	0.7660	0.066*
C4	0.43196 (11)	0.5436 (3)	0.9373 (3)	0.0514 (9)
C5	0.43624 (12)	0.4594 (3)	1.0321 (3)	0.0581 (10)
H5	0.4556	0.4797	1.1018	0.070*
C6	0.41236 (12)	0.3465 (3)	1.0248 (3)	0.0625 (10)
H6	0.4156	0.2915	1.0895	0.075*
C7	0.45454 (11)	0.6676 (3)	0.9520 (3)	0.0547 (9)
H7	0.4773	0.6811	1.0166	0.066*
C8	0.45321 (11)	0.9804 (3)	0.8454 (3)	0.0511 (9)
C9	0.41337 (12)	0.9737 (3)	0.7488 (3)	0.0630 (10)
H9A	0.3860	0.9767	0.7837	0.076*
H9B	0.4139	0.8920	0.7091	0.076*
C10	0.41111 (11)	1.0783 (4)	0.6579 (3)	0.0600 (10)
H10A	0.4149	1.1605	0.6975	0.072*
H10B	0.4357	1.0677	0.6132	0.072*
C11	0.36679 (11)	1.0763 (4)	0.5748 (3)	0.0614 (10)
H11A	0.3674	1.1358	0.5102	0.074*
H11B	0.3606	0.9913	0.5421	0.074*
C12	0.28823 (11)	1.1024 (3)	0.5954 (3)	0.0496 (9)

C13	0.27126 (12)	1.0486 (3)	0.4891 (3)	0.0565 (9)
H13	0.2908	1.0149	0.4418	0.068*
C14	0.22403 (13)	1.0442 (3)	0.4511 (3)	0.0622 (10)
H14	0.2127	1.0056	0.3791	0.075*
C15	0.19476 (13)	1.0945 (3)	0.5163 (4)	0.0626 (10)
H15	0.1637	1.0898	0.4893	0.075*
C16	0.21118 (11)	1.1545 (3)	0.6257 (3)	0.0533 (9)
C17	0.18326 (13)	1.2158 (4)	0.6962 (4)	0.0637 (10)
H17	0.1520	1.2164	0.6727	0.076*
C18	0.20197 (14)	1.2736 (4)	0.7978 (4)	0.0692 (11)
H18	0.1838	1.3153	0.8442	0.083*
C19	0.24899 (13)	1.2701 (4)	0.8326 (4)	0.0649 (10)
H19	0.2613	1.3097	0.9032	0.078*
C20	0.25844 (11)	1.1569 (3)	0.6668 (3)	0.0478 (8)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0747 (18)	0.0550 (16)	0.0739 (19)	−0.0169 (13)	−0.0058 (14)	0.0111 (13)
O2	0.0666 (17)	0.0543 (16)	0.0755 (18)	−0.0156 (13)	−0.0074 (14)	0.0019 (13)
O3	0.0481 (14)	0.0703 (17)	0.0613 (15)	0.0026 (12)	0.0039 (12)	−0.0158 (13)
O4	0.141 (4)	0.109 (4)	0.114 (4)	0.000	0.013 (3)	0.000
N1	0.0551 (18)	0.0462 (18)	0.066 (2)	−0.0064 (14)	0.0020 (15)	0.0010 (16)
N2	0.0522 (17)	0.0499 (18)	0.0643 (19)	−0.0096 (14)	−0.0059 (14)	0.0009 (15)
N3	0.0524 (17)	0.0484 (18)	0.064 (2)	−0.0031 (14)	0.0063 (15)	−0.0029 (15)
C1	0.055 (2)	0.043 (2)	0.064 (2)	−0.0017 (17)	0.0044 (19)	−0.0033 (18)
C2	0.063 (2)	0.048 (2)	0.051 (2)	−0.0030 (18)	−0.0009 (17)	−0.0008 (17)
C3	0.064 (2)	0.051 (2)	0.049 (2)	0.0007 (18)	0.0069 (18)	0.0058 (17)
C4	0.048 (2)	0.046 (2)	0.059 (2)	0.0013 (16)	0.0064 (17)	0.0016 (17)
C5	0.058 (2)	0.056 (2)	0.055 (2)	−0.0040 (18)	−0.0047 (18)	0.0017 (19)
C6	0.072 (2)	0.053 (2)	0.059 (2)	−0.006 (2)	0.001 (2)	0.0119 (19)
C7	0.048 (2)	0.051 (2)	0.063 (2)	−0.0026 (17)	0.0030 (17)	0.0003 (19)
C8	0.047 (2)	0.045 (2)	0.059 (2)	−0.0037 (17)	0.0026 (17)	−0.0004 (18)
C9	0.063 (2)	0.051 (2)	0.069 (2)	−0.0076 (18)	−0.008 (2)	0.0007 (19)
C10	0.050 (2)	0.068 (2)	0.063 (2)	−0.0010 (18)	0.0090 (18)	0.005 (2)
C11	0.061 (2)	0.062 (2)	0.061 (2)	0.0082 (19)	0.010 (2)	0.0068 (19)
C12	0.045 (2)	0.042 (2)	0.059 (2)	−0.0029 (15)	0.0014 (17)	−0.0001 (17)
C13	0.063 (2)	0.048 (2)	0.057 (2)	−0.0026 (17)	0.0042 (19)	−0.0045 (17)
C14	0.071 (3)	0.051 (2)	0.059 (2)	−0.0104 (19)	−0.008 (2)	−0.0001 (19)
C15	0.053 (2)	0.052 (2)	0.077 (3)	−0.0098 (18)	−0.007 (2)	0.007 (2)
C16	0.051 (2)	0.040 (2)	0.066 (2)	−0.0036 (16)	0.0009 (18)	0.0076 (18)
C17	0.050 (2)	0.057 (2)	0.083 (3)	0.0037 (18)	0.009 (2)	0.006 (2)
C18	0.065 (3)	0.064 (3)	0.080 (3)	0.009 (2)	0.018 (2)	−0.003 (2)
C19	0.068 (3)	0.060 (2)	0.066 (2)	0.004 (2)	0.012 (2)	−0.009 (2)
C20	0.052 (2)	0.0364 (19)	0.053 (2)	−0.0028 (15)	0.0026 (17)	0.0000 (16)

Geometric parameters (Å, °)

O1—C1	1.355 (4)	C8—C9	1.488 (5)

O1—H1	0.8200	C9—C10	1.505 (5)
O2—C8	1.238 (4)	C9—H9A	0.9700
O3—C12	1.362 (4)	C9—H9B	0.9700
O3—C11	1.432 (4)	C10—C11	1.499 (5)
O4—H20	0.8500	C10—H10A	0.9700
N1—C7	1.277 (4)	C10—H10B	0.9700
N1—N2	1.391 (4)	C11—H11A	0.9700
N2—C8	1.345 (4)	C11—H11B	0.9700
N2—H2	0.8600	C12—C13	1.362 (4)
N3—C19	1.308 (4)	C12—C20	1.424 (5)
N3—C20	1.368 (4)	C13—C14	1.408 (5)
C1—C6	1.383 (5)	C13—H13	0.9300
C1—C2	1.389 (5)	C14—C15	1.348 (5)
C2—C3	1.367 (5)	C14—H14	0.9300
C2—H2A	0.9300	C15—C16	1.416 (5)
C3—C4	1.394 (5)	C15—H15	0.9300
C3—H3	0.9300	C16—C17	1.408 (5)
C4—C5	1.389 (5)	C16—C20	1.414 (5)
C4—C7	1.459 (5)	C17—C18	1.349 (5)
C5—C6	1.376 (5)	C17—H17	0.9300
C5—H5	0.9300	C18—C19	1.397 (5)
C6—H6	0.9300	C18—H18	0.9300
C7—H7	0.9300	C19—H19	0.9300
C1—O1—H1	109.5	C9—C10—H10A	109.4
C12—O3—C11	119.6 (3)	C11—C10—H10B	109.4
C7—N1—N2	115.4 (3)	C9—C10—H10B	109.4
C8—N2—N1	121.0 (3)	H10A—C10—H10B	108.0
C8—N2—H2	119.5	O3—C11—C10	106.3 (3)
N1—N2—H2	119.5	O3—C11—H11A	110.5
C19—N3—C20	118.0 (3)	C10—C11—H11A	110.5
O1—C1—C6	118.5 (3)	O3—C11—H11B	110.5
O1—C1—C2	122.4 (3)	C10—C11—H11B	110.5
C6—C1—C2	119.1 (3)	H11A—C11—H11B	108.7
C3—C2—C1	120.2 (3)	O3—C12—C13	126.1 (3)
C3—C2—H2A	119.9	O3—C12—C20	113.7 (3)
C1—C2—H2A	119.9	C13—C12—C20	120.2 (3)
C2—C3—C4	121.4 (3)	C12—C13—C14	119.8 (3)
C2—C3—H3	119.3	C12—C13—H13	120.1
C4—C3—H3	119.3	C14—C13—H13	120.1
C5—C4—C3	117.7 (3)	C15—C14—C13	121.7 (4)
C5—C4—C7	119.5 (3)	C15—C14—H14	119.2
C3—C4—C7	122.8 (3)	C13—C14—H14	119.2
C6—C5—C4	121.2 (3)	C14—C15—C16	120.1 (3)
C6—C5—H5	119.4	C14—C15—H15	119.9
C4—C5—H5	119.4	C16—C15—H15	119.9
C5—C6—C1	120.3 (3)	C17—C16—C20	117.1 (3)
C5—C6—H6	119.9	C17—C16—C15	123.9 (3)
C1—C6—H6	119.9	C20—C16—C15	119.0 (3)
N1—C7—C4	121.2 (3)	C18—C17—C16	119.9 (3)

N1—C7—H7	119.4	C18—C17—H17	120.1
C4—C7—H7	119.4	C16—C17—H17	120.1
O2—C8—N2	119.6 (3)	C17—C18—C19	119.3 (4)
O2—C8—C9	122.2 (3)	C17—C18—H18	120.4
N2—C8—C9	118.1 (3)	C19—C18—H18	120.4
C8—C9—C10	114.8 (3)	N3—C19—C18	123.7 (4)
C8—C9—H9A	108.6	N3—C19—H19	118.2
C10—C9—H9A	108.6	C18—C19—H19	118.2
C8—C9—H9B	108.6	N3—C20—C16	122.0 (3)
C10—C9—H9B	108.6	N3—C20—C12	118.8 (3)
H9A—C9—H9B	107.5	C16—C20—C12	119.1 (3)
C11—C10—C9	111.3 (3)	H20—O4—H20Ai	105.8
C11—C10—H10A	109.4		
C7—N1—N2—C8	−167.8 (3)	C11—O3—C12—C20	−172.5 (3)
O1—C1—C2—C3	178.4 (3)	O3—C12—C13—C14	179.8 (3)
C6—C1—C2—C3	−2.3 (5)	C20—C12—C13—C14	−1.5 (5)
C1—C2—C3—C4	−1.0 (5)	C12—C13—C14—C15	1.4 (5)
C2—C3—C4—C5	3.9 (5)	C13—C14—C15—C16	0.4 (5)
C2—C3—C4—C7	−173.8 (3)	C14—C15—C16—C17	176.3 (3)
C3—C4—C5—C6	−3.5 (5)	C14—C15—C16—C20	−2.0 (5)
C7—C4—C5—C6	174.3 (3)	C20—C16—C17—C18	0.2 (5)
C4—C5—C6—C1	0.3 (6)	C15—C16—C17—C18	−178.2 (3)
O1—C1—C6—C5	−178.0 (3)	C16—C17—C18—C19	−1.0 (6)
C2—C1—C6—C5	2.7 (5)	C20—N3—C19—C18	0.6 (5)
N2—N1—C7—C4	178.6 (3)	C17—C18—C19—N3	0.6 (6)
C5—C4—C7—N1	−164.0 (3)	C19—N3—C20—C16	−1.4 (5)
C3—C4—C7—N1	13.7 (5)	C19—N3—C20—C12	176.2 (3)
N1—N2—C8—O2	175.1 (3)	C17—C16—C20—N3	1.0 (5)
N1—N2—C8—C9	−2.7 (5)	C15—C16—C20—N3	179.4 (3)
O2—C8—C9—C10	25.9 (5)	C17—C16—C20—C12	−176.5 (3)
N2—C8—C9—C10	−156.4 (3)	C15—C16—C20—C12	1.9 (5)
C8—C9—C10—C11	−171.3 (3)	O3—C12—C20—N3	1.1 (4)
C12—O3—C11—C10	−170.8 (3)	C13—C12—C20—N3	−177.8 (3)
C9—C10—C11—O3	68.2 (4)	O3—C12—C20—C16	178.7 (3)
C11—O3—C12—C13	6.3 (5)	C13—C12—C20—C16	−0.1 (5)

Symmetry codes: i.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N3^{i}	0.82	1.96	2.766 (4)	168
O4—H20···O2^{ii}	0.85	2.26	3.054 (5)	156
N2—H2···O2^{iii}	0.86	2.09	2.891 (4)	155

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

Fig. 1

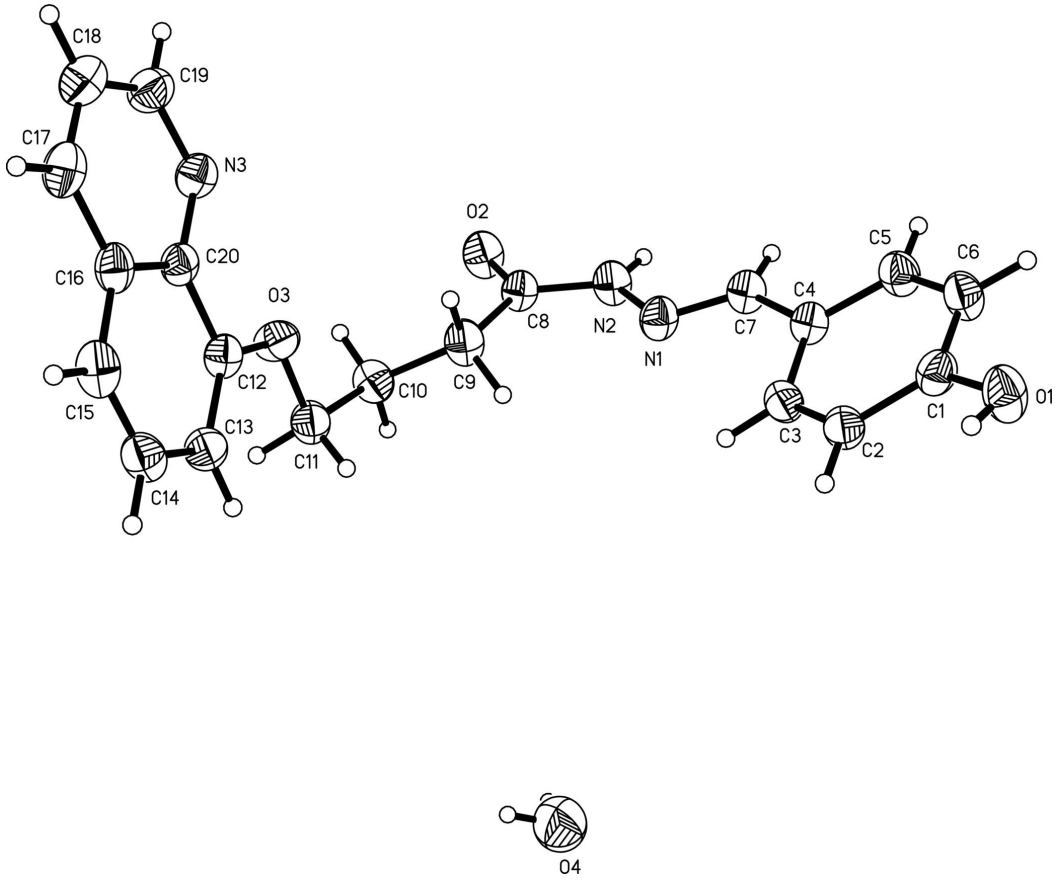
C18
C19
C17
N3
O2
C5
C6
C16
C20
O3
C8
N2
C7
C4
C12
C10
C9
N1
O1
C15
C13
C1
C3
C2
C11
C14
O4

Fig. 2