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4-Bromo-2-{[2-(2-hydroxybenzylideneamino)phenylimino]phenylmethyl}phenol

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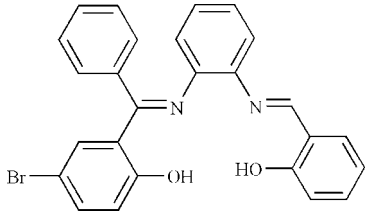
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; R factor = 0.034; wR factor = 0.091; data-to-parameter ratio = 12.9.

In the title compound, $C_{26}H_{19}BrN_2O_2$, all bond lengths and angles show normal values. Two hydroxy groups are involved in intramolecular O—H···N hydrogen bonds, which influence the molecular conformation. In the crystal structure, weak intermolecular C—H···O hydrogen bonds link the molecules into zigzag chains along the [101] direction.

Related literature

For related literature, see: Abu-Hussen (2006); Dale *et al.* (1999); Jurisson & Lydon (1999); Mladenova *et al.* (2002); Sanjay *et al.* (2004); Singh *et al.* (2006); Wiktor *et al.* (2000).



Experimental

Crystal data

$C_{26}H_{19}BrN_2O_2$
M_r = 471.34
Triclinic, $P\overline{1}$
a = 9.1682 (18) Å
b = 9.7011 (19) Å
c = 12.986 (3) Å
α = 90.87 (3)°
β = 108.79 (3)°
γ = 94.09 (3)°
V = 1089.8 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.91 mm^{-1}
T = 295 (2) K
0.25 × 0.20 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
4501 measured reflections
3742 independent reflections
2837 reflections with $I > 2\sigma(I)$
R_{int} = 0.018
3 standard reflections
every 100 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.091
S = 1.07
3742 reflections
289 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N2	0.80 (3)	1.79 (3)	2.530 (3)	154 (3)
O2—H2···N1	0.81 (3)	1.87 (3)	2.596 (3)	148 (3)
C2—H2C···O1^{i}	0.93	2.51	3.419 (4)	166
C15—H15A···O2^{ii}	0.93	2.60	3.497 (4)	162

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1990); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2333).

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supplementary materials

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4-Bromo-2-{[2-(2-hydroxybenzylideneamino)phenylimino]phenylmethyl}phenol

F. Yang, Y. Wang and Z. Zhang

Comment

Schiff bases exhibit often important biological activities such as antibacterial (Abu-Hussen *et al.*, 2006), antifungal (Singh *et al.*, 2006) and antitumor (Mladenova *et al.*, 2002). Radio-labeled (bio) molecules are potentially useful tools for cancer diagnosis and therapy. Many efforts have been made to develop diagnostic pharmaceuticals of 99mTc-labelled small molecular complexes because of the superior medico-imaging characteristics (biological t1/2, Low energy content) and the availability of radionuclide (Jurisson *et al.*, 1999). Since the small size of the complex is very important for the retention of the bioactivity, one of the strategies in the investigation is to explore novel complexes with small size, multifunctional ligands that possess specific bioactivities. Amino acids, mono/disaccharides and vitamins are good examples for these applications. Some applications of these Schiff bases with favorable cell membrane permeability have been exploited in cancer multidrug resistance (Jurisson *et al.*, 1999). We describe here the structure of the title compound.

In the title compound, bond lengths are slightly different from those in similar compounds. The C—Br bond length [1.905 (2) Å] is longer than others reported [1.865 (1) (Dale *et al.*, 1999) and 1.884 (2)Å (Wiktor *et al.*, 2000)]. The C—N bond lengths [1.276 (3) and 1.291 (3) Å] are shorter than that of 1.335 (2) Å reported by Sanjay *et al.* (2004). Two hydroxy groups are involved in intramolecular O—H···N hydrogen-bonding (Table 1).

The mean planes of the rings C1—C6 (P1), C8—C13 (P2), C14—C19 (P3) and C21—C26 (P4) make the following dihedral angles - P1/P4 78.3 (2)°, P2/P4 68.9 (4) and P3/P4 11.1 (2)°.

In the crystal, weak intermolecular C—H···O hydrogen bonds (Table 1) link the molecules into zigzag chains along direction [101].

Experimental

5-Bromo-2-hydroxybenzophenone (27.7 g, 0.1 mol), 1,2-diaminobenzene (10.8 g, 0.1 mol), piperidine (10.2 g, 0.12 mol) and triethylorthoformate (12 ml) were refluxed in absolute ethanol (120 ml) resulting in red-orange product of HBBP-PHEN. The title compound was prepared by the reaction of HBBP-PHEN (22.0 g, 0.06 mol), salicylaldehyde (12.2 g, 0.1 mol) with piperidine (10.2 g, 0.12 mol) at room temperature. The precipitated yellow solid was collected by filtration and washed twice with hot methanol. Single crystals suitable for X-ray measurements were obtained by recrystallization from absolute ethanol and acetic ether (1:1,*v*/*v*) at room temperature.

Refinement

C-bound H atoms were fixed geometrically (C—H 0.93 Å) and allowed to ride on their parent atoms, with U_{iso}(H)=1.2U_{eq}(C). Atoms H1 and H2 were located on difference map and refined isotropically with bond restraint O—H = 0.80 (3) Å.

Figures

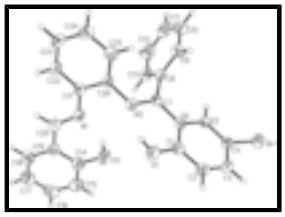

Fig. 1. The molecular structure of the title compound showing 30% probability displacement ellipsoids and the atom-numbering scheme.

4-Bromo-2-{[2-(2-hydroxybenzylideneamino)phenylimino]phenylmethyl}phenol

Crystal data

$C_{26}H_{19}BrN_2O_2$	$Z = 2$
$M_r = 471.34$	$F_{000} = 480$
Triclinic, $P\bar{1}$	$D_x = 1.436$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.1682$ (18) Å	Cell parameters from 25 reflections
$b = 9.7011$ (19) Å	$\theta = 4$–14º
$c = 12.986$ (3) Å	$\mu = 1.91$ mm^{-1}
$\alpha = 90.87$ (3)º	$T = 295$ (2) K
$\beta = 108.79$ (3)º	Block, colourless
$\gamma = 94.09$ (3)º	0.25 × 0.20 × 0.20 mm
$V = 1089.8$ (4) Å^3	

Data collection

Enraf–Nonius CAD-4 diffractometer	$R_{int} = 0.018$
Radiation source: fine-focus sealed tube	$\theta_{max} = 25.0$º
Monochromator: graphite	$\theta_{min} = 1.7$º
$T = 295(2)$ K	$h = -10 \rightarrow 10$
ω scans	$k = -11 \rightarrow 7$
Absorption correction: none	$l = -15 \rightarrow 12$
4501 measured reflections	3 standard reflections
3742 independent reflections	every 100 reflections
2837 reflections with $I > 2\sigma(I)$	intensity decay: none

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.034$	$w = 1/[\sigma^2(F_o^2) + (0.0443P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$wR(F^2) = 0.091$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.07$	$\Delta\rho_{max} = 0.26$ e Å^{-3}
3742 reflections	$\Delta\rho_{min} = -0.30$ e Å^{-3}
289 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0051 (14)
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 $F^2 > 2\text{sigma}(F^2)$ 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}
Br1	0.10044 (3)	0.19363 (3)	0.02361 (3)	0.06928 (16)
O1	−0.4811 (3)	0.3545 (2)	0.0968 (2)	0.0759 (7)
O2	−0.2232 (3)	0.3849 (3)	0.4416 (2)	0.0907 (8)
N1	−0.4694 (3)	0.2214 (2)	0.41956 (17)	0.0535 (6)
N2	−0.4777 (3)	0.1461 (2)	0.21221 (16)	0.0518 (5)
C1	−0.3534 (3)	0.3110 (3)	0.0812 (2)	0.0536 (7)
C2	−0.2881 (3)	0.3884 (3)	0.0147 (2)	0.0619 (8)
H2C	−0.3349	0.4655	−0.0183	0.074*
C3	−0.1559 (3)	0.3518 (3)	−0.0024 (2)	0.0562 (7)
H3A	−0.1128	0.4043	−0.0462	0.067*
C4	−0.0870 (3)	0.2371 (3)	0.0456 (2)	0.0474 (6)
C5	−0.1511 (3)	0.1557 (3)	0.10858 (19)	0.0462 (6)
H5A	−0.1042	0.0773	0.1389	0.055*
C6	−0.2872 (3)	0.1906 (2)	0.12716 (18)	0.0436 (6)
C7	−0.3600 (3)	0.1023 (3)	0.19163 (18)	0.0442 (6)
C8	−0.2987 (3)	−0.0321 (3)	0.2296 (2)	0.0487 (6)
C9	−0.3297 (4)	−0.1462 (3)	0.1588 (3)	0.0759 (9)
H9A	−0.3842	−0.1378	0.0855	0.091*
C10	−0.2800 (5)	−0.2733 (4)	0.1967 (4)	0.0986 (13)
H10A	−0.3017	−0.3502	0.1491	0.118*
C11	−0.1981 (5)	−0.2849 (4)	0.3055 (4)	0.1011 (14)
H11A	−0.1650	−0.3700	0.3312	0.121*
C12	−0.1656 (4)	−0.1727 (4)	0.3750 (3)	0.0879 (11)
H12A	−0.1094	−0.1811	0.4480	0.106*

C13	−0.2157 (3)	−0.0453 (3)	0.3376 (2)	0.0647 (8)
H13A	−0.1932	0.0312	0.3857	0.078*
C14	−0.2425 (4)	0.4371 (3)	0.5333 (2)	0.0647 (8)
C15	−0.1351 (4)	0.5408 (3)	0.5954 (3)	0.0794 (9)
H15A	−0.0526	0.5739	0.5733	0.095*
C16	−0.1522 (4)	0.5937 (3)	0.6893 (3)	0.0823 (10)
H16A	−0.0805	0.6626	0.7304	0.099*
C17	−0.2734 (4)	0.5464 (4)	0.7236 (3)	0.0815 (10)
H17A	−0.2829	0.5829	0.7875	0.098*
C18	−0.3795 (4)	0.4459 (3)	0.6633 (2)	0.0716 (9)
H18A	−0.4617	0.4147	0.6864	0.086*
C19	−0.3663 (3)	0.3888 (3)	0.5670 (2)	0.0546 (7)
C20	−0.4790 (3)	0.2801 (3)	0.5055 (2)	0.0580 (7)
H20A	−0.5612	0.2521	0.5296	0.070*
C21	−0.5766 (3)	0.1108 (3)	0.3638 (2)	0.0495 (6)
C22	−0.6821 (3)	0.0394 (3)	0.4052 (2)	0.0671 (8)
H22A	−0.6867	0.0666	0.4730	0.081*
C23	−0.7793 (3)	−0.0705 (3)	0.3476 (3)	0.0684 (8)
H23A	−0.8508	−0.1147	0.3756	0.082*
C24	−0.7710 (3)	−0.1143 (3)	0.2498 (2)	0.0647 (8)
H24A	−0.8352	−0.1896	0.2118	0.078*
C25	−0.6669 (3)	−0.0467 (3)	0.2071 (2)	0.0617 (7)
H25A	−0.6617	−0.0770	0.1401	0.074*
C26	−0.5700 (3)	0.0657 (3)	0.2628 (2)	0.0474 (6)
H1	−0.500 (4)	0.301 (3)	0.139 (3)	0.080 (11)*
H2	−0.290 (4)	0.323 (4)	0.415 (3)	0.105 (14)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0561 (2)	0.0758 (3)	0.0844 (3)	0.00471 (15)	0.03481 (16)	−0.00113 (17)
O1	0.0859 (16)	0.0664 (15)	0.1017 (17)	0.0342 (12)	0.0595 (14)	0.0357 (13)
O2	0.0899 (17)	0.1015 (19)	0.0897 (17)	−0.0397 (16)	0.0532 (14)	−0.0303 (15)
N1	0.0595 (14)	0.0516 (14)	0.0530 (13)	−0.0048 (11)	0.0252 (11)	0.0004 (11)
N2	0.0615 (14)	0.0484 (13)	0.0531 (12)	0.0059 (11)	0.0288 (11)	0.0048 (10)
C1	0.0584 (16)	0.0456 (16)	0.0644 (17)	0.0116 (13)	0.0288 (14)	0.0078 (13)
C2	0.074 (2)	0.0489 (17)	0.0747 (19)	0.0162 (15)	0.0370 (16)	0.0188 (15)
C3	0.0667 (18)	0.0491 (17)	0.0593 (16)	−0.0040 (14)	0.0309 (14)	0.0064 (14)
C4	0.0466 (14)	0.0464 (15)	0.0495 (14)	0.0015 (12)	0.0169 (12)	−0.0028 (12)
C5	0.0523 (15)	0.0406 (14)	0.0461 (14)	0.0041 (12)	0.0166 (12)	−0.0003 (12)
C6	0.0509 (14)	0.0400 (14)	0.0414 (13)	0.0035 (12)	0.0172 (11)	0.0005 (11)
C7	0.0506 (15)	0.0432 (14)	0.0391 (13)	0.0002 (12)	0.0161 (11)	−0.0048 (11)
C8	0.0547 (15)	0.0456 (16)	0.0546 (16)	0.0063 (13)	0.0290 (13)	0.0078 (13)
C9	0.100 (3)	0.0517 (19)	0.080 (2)	0.0100 (18)	0.0338 (19)	0.0046 (17)
C10	0.130 (3)	0.049 (2)	0.142 (4)	0.015 (2)	0.078 (3)	0.008 (2)
C11	0.113 (3)	0.083 (3)	0.146 (4)	0.044 (3)	0.087 (3)	0.056 (3)
C12	0.081 (2)	0.107 (3)	0.093 (3)	0.037 (2)	0.044 (2)	0.052 (3)
C13	0.0644 (18)	0.074 (2)	0.0624 (18)	0.0141 (16)	0.0278 (15)	0.0177 (16)

C14	0.0684 (19)	0.0620 (19)	0.0627 (18)	−0.0044 (16)	0.0221 (15)	−0.0041 (15)
C15	0.069 (2)	0.075 (2)	0.090 (2)	−0.0137 (18)	0.0232 (18)	−0.006 (2)
C16	0.088 (3)	0.065 (2)	0.074 (2)	−0.0004 (19)	0.0017 (19)	−0.0128 (18)
C17	0.093 (3)	0.077 (2)	0.068 (2)	0.007 (2)	0.0176 (19)	−0.0120 (18)
C18	0.082 (2)	0.067 (2)	0.0681 (19)	0.0057 (18)	0.0270 (17)	−0.0061 (17)
C19	0.0590 (17)	0.0490 (16)	0.0559 (16)	0.0049 (14)	0.0184 (13)	0.0025 (14)
C20	0.0591 (17)	0.0592 (18)	0.0609 (17)	0.0014 (14)	0.0273 (14)	0.0044 (15)
C21	0.0500 (15)	0.0480 (16)	0.0546 (15)	0.0036 (13)	0.0226 (13)	0.0033 (13)
C22	0.076 (2)	0.070 (2)	0.0663 (18)	−0.0111 (17)	0.0420 (16)	−0.0019 (16)
C23	0.0593 (18)	0.068 (2)	0.085 (2)	−0.0085 (16)	0.0358 (16)	0.0062 (17)
C24	0.0604 (18)	0.0603 (19)	0.0660 (18)	−0.0094 (15)	0.0132 (15)	0.0002 (15)
C25	0.0691 (19)	0.0618 (19)	0.0517 (16)	−0.0018 (16)	0.0179 (14)	−0.0012 (14)
C26	0.0474 (15)	0.0470 (15)	0.0514 (15)	0.0067 (12)	0.0200 (12)	0.0096 (13)

Geometric parameters (Å, °)

Br1—C4	1.905 (2)	C12—C13	1.389 (4)
O1—C1	1.346 (3)	C12—H12A	0.9300
O1—H1	0.80 (3)	C13—H13A	0.9300
O2—C14	1.354 (3)	C14—C19	1.397 (4)
O2—H2	0.81 (3)	C14—C15	1.398 (4)
N1—C20	1.276 (3)	C15—C16	1.375 (4)
N1—C21	1.418 (3)	C15—H15A	0.9300
N2—C7	1.291 (3)	C16—C17	1.377 (5)
N2—C26	1.427 (3)	C16—H16A	0.9300
C1—C2	1.399 (4)	C17—C18	1.364 (4)
C1—C6	1.406 (3)	C17—H17A	0.9300
C2—C3	1.370 (4)	C18—C19	1.404 (4)
C2—H2C	0.9300	C18—H18A	0.9300
C3—C4	1.376 (4)	C19—C20	1.451 (4)
C3—H3A	0.9300	C20—N1	1.276 (3)
C4—C5	1.379 (3)	C20—H20A	0.9300
C5—C6	1.407 (3)	C21—C22	1.398 (3)
C5—H5A	0.9300	C21—C26	1.398 (3)
C6—C7	1.477 (3)	C21—N1	1.418 (3)
C7—N2	1.291 (3)	C22—C23	1.379 (4)
C7—C8	1.485 (4)	C22—H22A	0.9300
C8—C13	1.377 (4)	C23—C24	1.359 (4)
C8—C9	1.380 (4)	C23—H23A	0.9300
C9—C10	1.387 (5)	C24—C25	1.383 (4)
C9—H9A	0.9300	C24—H24A	0.9300
C10—C11	1.381 (6)	C25—C26	1.388 (4)
C10—H10A	0.9300	C25—H25A	0.9300
C11—C12	1.355 (5)	C26—N2	1.427 (3)
C11—H11A	0.9300		
C1—O1—H1	104 (2)	O2—C14—C19	121.4 (3)
C14—O2—H2	110 (3)	O2—C14—C15	118.9 (3)
C20—N1—C21	121.4 (2)	C19—C14—C15	119.7 (3)
C7—N2—C26	123.7 (2)	C16—C15—C14	119.6 (3)

O1—C1—C2	117.7 (2)	C16—C15—H15A	120.2
O1—C1—C6	122.4 (2)	C14—C15—H15A	120.2
C2—C1—C6	119.9 (2)	C15—C16—C17	121.2 (3)
C3—C2—C1	120.7 (3)	C15—C16—H16A	119.4
C3—C2—H2C	119.6	C17—C16—H16A	119.4
C1—C2—H2C	119.6	C18—C17—C16	119.7 (3)
C2—C3—C4	119.7 (2)	C18—C17—H17A	120.1
C2—C3—H3A	120.1	C16—C17—H17A	120.1
C4—C3—H3A	120.1	C17—C18—C19	120.9 (3)
C3—C4—C5	121.1 (2)	C17—C18—H18A	119.5
C3—C4—Br1	118.32 (19)	C19—C18—H18A	119.5
C5—C4—Br1	120.6 (2)	C14—C19—C18	118.8 (3)
C4—C5—C6	120.3 (2)	C14—C19—C20	121.3 (2)
C4—C5—H5A	119.8	C18—C19—C20	119.9 (3)
C6—C5—H5A	119.8	N1—C20—C19	122.4 (2)
C1—C6—C5	118.1 (2)	N1—C20—C19	122.4 (2)
C1—C6—C7	120.8 (2)	N1—C20—H20A	118.8
C5—C6—C7	121.1 (2)	N1—C20—H20A	118.8
N2—C7—C6	117.6 (2)	C19—C20—H20A	118.8
N2—C7—C6	117.6 (2)	C22—C21—C26	118.0 (2)
N2—C7—C8	122.2 (2)	C22—C21—N1	124.7 (2)
N2—C7—C8	122.2 (2)	C26—C21—N1	117.2 (2)
C6—C7—C8	120.2 (2)	C22—C21—N1	124.7 (2)
C13—C8—C9	119.3 (3)	C26—C21—N1	117.2 (2)
C13—C8—C7	119.8 (2)	C23—C22—C21	121.3 (3)
C9—C8—C7	120.8 (2)	C23—C22—H22A	119.4
C8—C9—C10	120.3 (3)	C21—C22—H22A	119.3
C8—C9—H9A	119.9	C24—C23—C22	120.2 (3)
C10—C9—H9A	119.9	C24—C23—H23A	119.9
C11—C10—C9	119.6 (4)	C22—C23—H23A	119.9
C11—C10—H10A	120.2	C23—C24—C25	119.9 (3)
C9—C10—H10A	120.2	C23—C24—H24A	120.1
C12—C11—C10	120.3 (4)	C25—C24—H24A	120.1
C12—C11—H11A	119.8	C24—C25—C26	120.8 (3)
C10—C11—H11A	119.8	C24—C25—H25A	119.6
C11—C12—C13	120.3 (4)	C26—C25—H25A	119.6
C11—C12—H12A	119.8	C25—C26—C21	119.7 (2)
C13—C12—H12A	119.8	C25—C26—N2	120.5 (2)
C8—C13—C12	120.1 (3)	C21—C26—N2	119.3 (2)
C8—C13—H13A	119.9	C25—C26—N2	120.5 (2)
C12—C13—H13A	119.9	C21—C26—N2	119.3 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N2	0.80 (3)	1.79 (3)	2.530 (3)	154 (3)
O2—H2···N1	0.81 (3)	1.87 (3)	2.596 (3)	148 (3)
C2—H2C···O1^{i}	0.93	2.51	3.419 (4)	166
C15—H15A···O2^{ii}	0.93	2.60	3.497 (4)	162

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

Fig. 1