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Crystal structure of 3-(4-hydroxyphenyl)-2-[(*E*)-2-phenylethenyl]quinazolin-4(3*H*)-one

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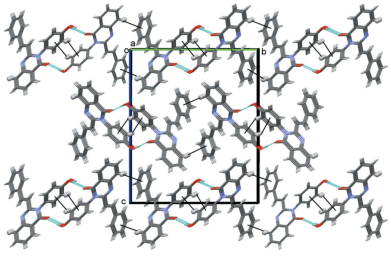
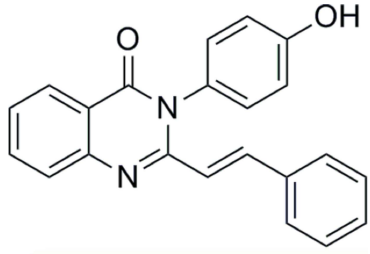
The title compound, $C_{22}H_{16}N_2O_2$ {systematic name: 3-(4-hydroxyphenyl)-2-[(*E*)-2-phenylethenyl]quinazolin-4(3*H*)-one}, consists of a substituted 2-[(*E*)-2-arylethenyl]-3-arylquinazolin-4(3*H*)-one skeleton. The substituents at the ethylene fragment are located in *trans* positions. The phenyl ring is inclined to the quinazolone ring by 26.44 (19)°, while the 4-hydroxyphenyl ring is inclined to the quinazolone ring by 81.25 (8)°. The phenyl ring and the 4-hydroxyphenyl ring are inclined to one another by 78.28 (2)°. In the crystal, molecules are connected *via* O—H···O hydrogen bonds, forming a helix along the *a*-axis direction. The helices are linked by C—H···π interactions, forming slabs parallel to (001).

1. Chemical context

Compounds containing the 2-[(*E*)-2-arylethenyl]-3-aryl-quinazolin-4(3*H*)-one core are well known for their broad biological activities. These compounds demonstrate antibiotic effect *in vivo* against methicillin-resistant *Staphylococcus aureus* (Bouley *et al.*, 2015; Chang *et al.*, 2014) and anti-leishmanial activity (Birhan *et al.*, 2014). 2-Styryl functionalized quinazolinones are applicable as anticancer agents against human cell lines (Kamal *et al.*, 2013; 2012; 2010*a*,*b*) and anticonvulsants (Das *et al.*, 2014). Analogues of the title compound are Hsp90 inhibitors with *in vitro* anti-tumor activity (Park *et al.*, 2007), as well as suppressants of the ubiquitin ligase activity of a human polypeptide (Erez & Nakache, 2011), GluN2D-containing NMDA receptors (Hansen & Traynelis, 2011) and c-KIT expression (Wang *et al.*, 2013). Compounds with such a structure are good modulators of both γ-secretase (Fischer *et al.*, 2011) and Rho C activity (Sun *et al.*, 2003), as well as AMPA receptor antagonists (Chenard *et al.*, 2001; 1999; Welch & DeVries, 1998). Piriqualone (the 2-hetarylvinyl analogue of the above mentioned compounds) has been used as a sedative–hypnotic drug (Kumar *et al.*, 2015).





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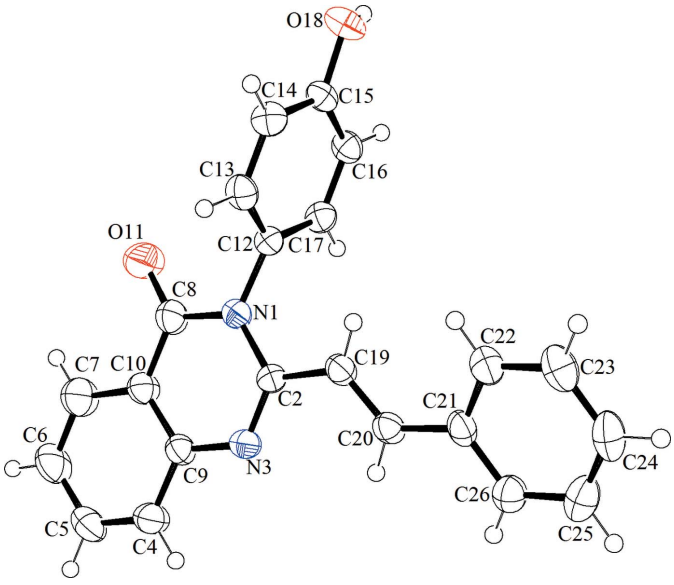

Figure 1
The molecular structure of compound **1**, showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

2. Structural commentary

The title compound **1**, Fig. 1, consists of a substituted 2-[(*E*)-2-arylethenyl]-3-arylquinazolin-4(3*H*)-one skeleton. The substituents at the ethylene fragment are located in *trans*-positions. Unlike the structure reported by Nosova *et al.* (2012), where the conjugation system of styrylquinazolinone is practically planar, in compound **1** the 2-phenyleth-(*E*)-enyl substituent is twisted with respect to the plane of the quinazolone ring. The phenyl (C21–C26) and the 4-hydroxyphenyl (C12–C17) rings are inclined to one another by 78.2 (2)°, and to the quinazolone ring (N1/N2/C2/C4–C10) by 26.44 (19) and 81.25 (8)°, respectively. A similar styrylquinazolinone conjugation system geometry has been found in structures reported previously (Trashakhova *et al.*, 2011; Ovchinnikova *et al.*, 2014).

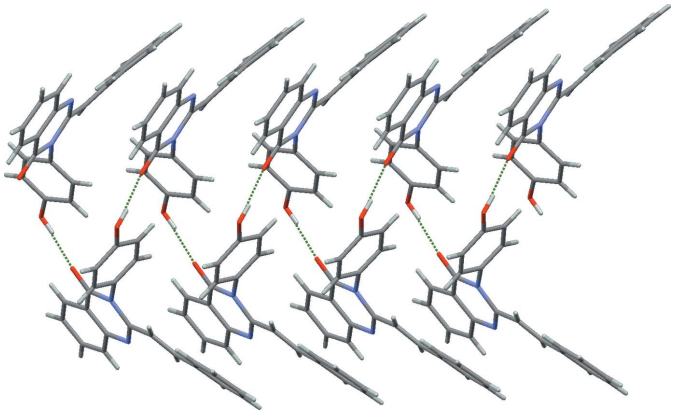

Figure 2
A fragment of the crystal structure of compound **1**, showing the helix-like hydrogen-bonded chain propagating along the *a*-axis direction.

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

*Cg*3 and *Cg*4 are the centroids of the C12–C17 and C21–C26 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O18—H18···O11^{i}	0.82	1.84	2.654 (5)	172
C4—H4···*Cg*4^{ii}	0.94	2.96	3.829 (5)	157
C16—H16···*Cg*3^{i}	0.94	2.95	3.646 (5)	133

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

3. Supramolecular features

In the crystal of **1**, molecules are connected *via* O—H···O hydrogen bonds forming a 2_1 helix, with graph set *C*(3), propagating along the *a*-axis direction (Table 1 and Fig. 2). This is similar to the crystal packing reported for the structure of diltiazem acetylsalicilate hydrate (Stepanovs *et al.*, 2016). In **1**, the helices are linked *via* C—H···π interactions, forming slabs lying parallel to the *ab* plane (Table 1 and Fig. 3).

4. Database survey

A search of the Cambridge Structural Database (Version 5.37; Groom & Allen, 2014) for substructure **S1** (Fig. 4) gave 137 hits, while a search for substructure **S2** (2-arylvinyl 3-aryl quinazolin-4(3*H*)-one skeleton, Fig. 4) gave only three hits: Nosova *et al.* (2012); Trashakhova *et al.* (2011); Ovchinnikova *et al.* (2014). However, none of the characterized single crystals contains a hydrogen-bond donor/acceptor in the aryl substituent at position 3 of the quinazolinone unit and information on intermolecular interactions of such structures is still missing. The only example containing a carboxylic functionality at the 3-aryl substituent of quinazolin-4(3*H*)-one was analysed as a complex with *Staphylococcus aureus* at the PBP2a binding site (Bouley *et al.*, 2015).

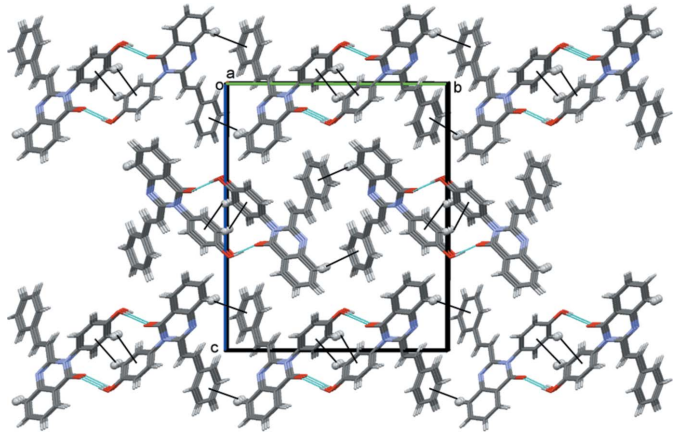

Figure 3
A view along the *a* axis of the crystal packing of compound **1**. The hydrogen bonds are shown as dashed lines and the C—H···π interactions (see Table 1) are represented as thin black lines.

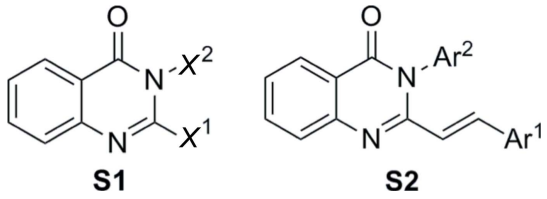

Figure 4
Substructures used for the Database survey.

5. Synthesis and crystallization

The title compound **1** was synthesized applying two pathways starting from 2-methyl (**2**) or 2-styryl (**3**) benzoxazin-4-one (methods *A* and *B*, respectively, Fig. 5).

Method A

2-Methyl benzoxazin-4-one (**2**) (0.263 g, 1.6 mmol) and 4-aminophenol (**4**) (0.175 g, 1.6 mmol) in glacial acetic acid (2 ml) were refluxed for 7 h, then poured into crushed ice (50 ml) and filtered. Compound **5** was obtained as a greyish solid. Its spectroscopic data corresponded to those in the literature (Marinho & Proença, 2015). The crude product **5**, without further purification, was subjected to condensation with benzaldehyde analogously to a known method (Krastina *et al.*, 2014): 3-(4-hydroxyphenyl)-2-methylquinazolin-4(3*H*)-one (**5**) (0.276 g, 1.1 mmol), benzaldehyde (0.27 g, 2.53 mol) and acetanhydride (0.5 ml) in acetic acid (4 ml) were refluxed for 8 h, poured into crushed ice (50 ml), filtered and air-dried. The mixture containing compounds **1** and **6** (0.25 g) was refluxed for 7 h in NaOH/methanol (5%, 5 ml), poured into crushed ice (50 ml), acidified with conc. hydrochloric acid and filtered. The target compound **1** was obtained as a white solid with 53% (0.197 g) yield over two steps.

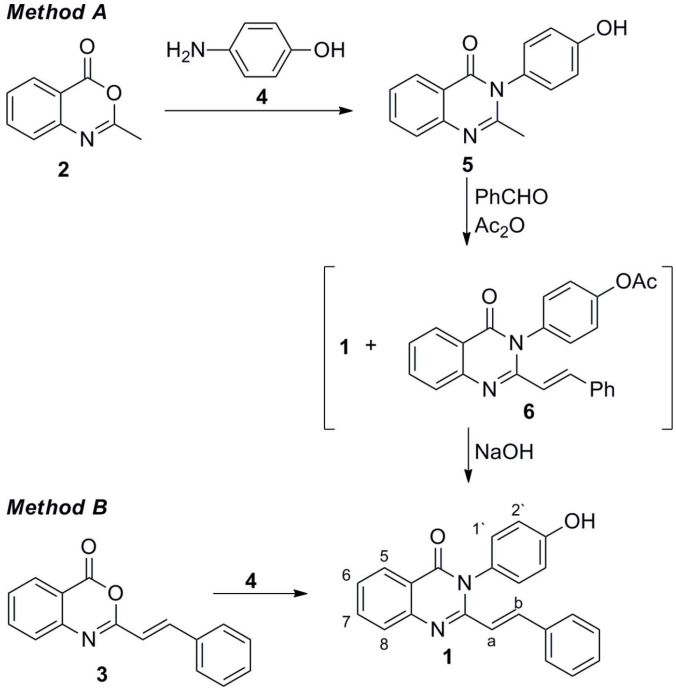

Figure 5
Synthesis of the title compound, **1**.

Method B

The title compound **1** was obtained as a by-product during the synthesis of 2-cinnamamido-*N*-(4-hydroxyphenyl)benzamide: benzoxazin-4-one **3** (1.00 g, 4 mmol) and 4-aminophenol (**4**) (0.44 g, 4 mmol) were refluxed in toluene (5 ml) for 3 h, then the mixture was filtered. The title compound was isolated by crystallization from ethanol.

Single crystals suitable for X-ray analysis were obtained by slow evaporation from ethanol at room temperature (m.p. > 523 K).

Spectroscopic data: IR (KBr), ν, cm^{-1}: 3300 (OH), 1655 (CON), 1150, 1515, 1470, 1450, 1340, 1225, 970, 775, 965. ^{1}H NMR (300 MHz, DMSO-d_6), δ (p.p.m.): 9.91 (1H, *s*, OH), 8.12 (1H, *d*, J = 7.8 Hz, H-5), 7.91–7.83 (2H, *m*, H-b, H-6/7), 7.76 (1H, *d*, J = 7.8 Hz, H-8), 7.52 (1H, *t*, J = 7.8 Hz, H-6/7), 7.41–7.33 (5H, *m*, Ph), 7.23 (2H, *d*, J = 8.6 Hz, H-1′), 6.94 (2H, *d*, J = 8.6 Hz, H-2′), 6.42 (1H, *d*, J = 15.4 Hz, H-a). ^{13}C NMR (75 MHz, DMSO-d_6), δ (p.p.m.): 161.5, 157.8, 152.0, 147.4, 138.6, 134.9, 134.7, 129.9, 129.8, 129.1, 127.9, 127.4, 127.1, 126.52, 126.47, 120.6, 120.2, 116.1. HRMS. Calculated $[M+H]^+$, m/z: 341.1285. $C_{22}H_{16}N_2O_2$. Found, m/z: 341.1282.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{22}H_{16}N_2O_2$
M_r	340.37
Crystal system, space group	Orthorhombic, $P2_1nb$
Temperature (K)	173
a, b, c (Å)	5.3469 (2), 16.5139 (6), 19.8885 (10)
V (Å^3)	1756.12 (13)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.22 × 0.18 × 0.09
Data collection	
Diffractometer	Nonius KappaCCD
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	3862, 3862, 2236
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.649
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.068, 0.139, 1.03
No. of reflections	3862
No. of parameters	236
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.17, −0.19

Computer programs: *KappaCCD Server Software* (Nonius, 1997), *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997), *SIR2011* (Burla *et al.*, 2012), *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2008), *SHELXL2015* (Sheldrick, 2015), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The C-bound H atoms were positioned geometrically and refined as riding on their parent

atoms: C—H = 0.93 − 0.98 Å with U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and 1.2U_{eq}(C) for other H atoms. The H atom of the hydroxyl group was included in the position identified from a difference Fourier map and was then refined as riding: O—H = 0.82 Å with U_{iso}(H) = 1.5U_{eq}(O).

Acknowledgements

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supporting information

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Computing details

Data collection: *KappaCCD Server Software* (Nonius, 1997); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR2011* (Burla *et al.*, 2012); program(s) used to refine structure: *SHELXL2015* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL2015* (Sheldrick, 2015), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

3-(4-Hydroxyphenyl)-2-[(*E*)-2-phenylethenyl]quinazolin-4(3*H*)-one

Crystal data

$C_{22}H_{16}N_2O_2$
$M_r = 340.37$
Orthorhombic, $P2_1nb$
$a = 5.3469$ (2) Å
$b = 16.5139$ (6) Å
$c = 19.8885$ (10) Å
$V = 1756.12$ (13) Å^3
$Z = 4$
$F(000) = 712$
$D_x = 1.287$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6856 reflections
$\theta = 1.0$–$27.5°$
$\mu = 0.08$ mm^{-1}
$T = 173$ K
Plate, colorless
0.22 × 0.18 × 0.09 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
φ and ω scan
3862 measured reflections
3862 independent reflections
2236 reflections with $I > 2\sigma(I)$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.2°$
$h = -6 \rightarrow 6$
$k = -21 \rightarrow 21$
$l = -25 \rightarrow 25$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.068$
$wR(F^2) = 0.139$
$S = 1.03$
3862 reflections
236 parameters
1 restraint
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0478P)^2 + 0.3939P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.6956 (7)	0.7742 (2)	0.45545 (18)	0.0333 (9)
C2	0.8449 (8)	0.7044 (3)	0.4584 (2)	0.0317 (10)
N3	0.8479 (7)	0.6500 (2)	0.41192 (18)	0.0372 (9)
C4	0.6912 (9)	0.6013 (3)	0.3061 (2)	0.0436 (12)
H4	0.7956	0.5564	0.3096	0.052*
C5	0.5358 (9)	0.6089 (3)	0.2518 (2)	0.0476 (13)
H5	0.5349	0.5690	0.2188	0.057*
C6	0.3791 (11)	0.6756 (3)	0.2457 (3)	0.0564 (15)
H6	0.2738	0.6801	0.2086	0.068*
C7	0.3795 (12)	0.7346 (3)	0.2939 (3)	0.0588 (15)
H7	0.2750	0.7793	0.2895	0.071*
C8	0.5362 (10)	0.7885 (3)	0.4018 (3)	0.0435 (12)
C9	0.6946 (8)	0.6604 (3)	0.3564 (2)	0.0337 (11)
C10	0.5376 (9)	0.7278 (3)	0.3501 (2)	0.0372 (11)
O11	0.4054 (7)	0.8506 (2)	0.40120 (19)	0.0653 (12)
C12	0.7042 (8)	0.8360 (3)	0.5076 (2)	0.0315 (10)
C13	0.5181 (8)	0.8382 (3)	0.5557 (2)	0.0354 (11)
H13	0.3953	0.7983	0.5563	0.042*
C14	0.5143 (9)	0.8993 (3)	0.6027 (2)	0.0372 (11)
H14	0.3905	0.9002	0.6356	0.045*
C15	0.6941 (8)	0.9595 (3)	0.6013 (2)	0.0309 (10)
C16	0.8821 (8)	0.9566 (3)	0.5533 (2)	0.0344 (11)
H16	1.0059	0.9962	0.5528	0.041*
C17	0.8859 (8)	0.8951 (3)	0.5064 (2)	0.0339 (11)
H17	1.0110	0.8936	0.4739	0.041*
O18	0.6763 (7)	1.01968 (18)	0.64797 (15)	0.0426 (8)
H18	0.7583	1.0589	0.6356	0.064*
C19	0.9961 (7)	0.6928 (3)	0.5188 (2)	0.0338 (11)
H19	0.9602	0.7230	0.5570	0.041*
C20	1.1845 (8)	0.6398 (3)	0.5204 (2)	0.0341 (10)
H20	1.2220	0.6133	0.4804	0.041*
C21	1.3390 (9)	0.6191 (3)	0.5794 (2)	0.0361 (11)
C22	1.2883 (9)	0.6474 (3)	0.6437 (2)	0.0435 (12)
H22	1.1527	0.6816	0.6508	0.052*
C23	1.4371 (8)	0.6252 (3)	0.6973 (3)	0.0498 (15)
H23	1.4006	0.6441	0.7402	0.060*
C24	1.6404 (9)	0.5748 (3)	0.6875 (3)	0.0512 (14)
H24	1.7421	0.5605	0.7235	0.061*
C25	1.6909 (10)	0.5460 (3)	0.6243 (3)	0.0496 (13)

H25	1.8265	0.5117	0.6176	0.060*
C26	1.5421 (9)	0.5676 (3)	0.5706 (2)	0.0399 (12)
H26	1.5779	0.5475	0.5280	0.048*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0351 (19)	0.030 (2)	0.035 (2)	0.0014 (17)	−0.0054 (19)	−0.0034 (17)
C2	0.031 (2)	0.027 (2)	0.037 (3)	0.003 (2)	−0.004 (2)	−0.002 (2)
N3	0.041 (2)	0.033 (2)	0.037 (2)	0.0064 (18)	−0.0066 (19)	−0.0067 (19)
C4	0.050 (3)	0.038 (3)	0.042 (3)	0.003 (2)	−0.001 (3)	−0.007 (2)
C5	0.052 (3)	0.051 (4)	0.040 (3)	−0.011 (3)	−0.001 (3)	−0.013 (3)
C6	0.066 (3)	0.065 (4)	0.038 (3)	−0.002 (3)	−0.017 (3)	−0.007 (3)
C7	0.067 (3)	0.059 (4)	0.050 (3)	0.012 (3)	−0.021 (3)	−0.003 (3)
C8	0.045 (3)	0.041 (3)	0.043 (3)	0.004 (3)	−0.012 (3)	−0.001 (2)
C9	0.036 (2)	0.034 (3)	0.031 (3)	−0.001 (2)	−0.004 (2)	−0.002 (2)
C10	0.044 (2)	0.038 (3)	0.030 (3)	0.004 (2)	−0.006 (2)	−0.001 (2)
O11	0.081 (3)	0.055 (3)	0.060 (3)	0.029 (2)	−0.030 (2)	−0.010 (2)
C12	0.031 (2)	0.031 (3)	0.032 (3)	0.003 (2)	−0.003 (2)	−0.003 (2)
C13	0.036 (2)	0.029 (3)	0.041 (3)	−0.009 (2)	−0.001 (2)	0.004 (2)
C14	0.039 (2)	0.037 (3)	0.036 (3)	−0.002 (2)	0.006 (2)	0.003 (2)
C15	0.040 (2)	0.027 (3)	0.026 (2)	−0.003 (2)	−0.003 (2)	0.001 (2)
C16	0.034 (2)	0.033 (3)	0.036 (3)	−0.007 (2)	0.001 (2)	0.000 (2)
C17	0.032 (2)	0.036 (3)	0.034 (3)	−0.001 (2)	0.004 (2)	0.001 (2)
O18	0.062 (2)	0.0355 (19)	0.0304 (17)	−0.0100 (17)	0.0041 (16)	−0.0058 (16)
C19	0.038 (2)	0.029 (3)	0.034 (3)	−0.002 (2)	−0.006 (2)	−0.002 (2)
C20	0.040 (2)	0.027 (2)	0.035 (3)	−0.002 (2)	−0.005 (2)	0.000 (2)
C21	0.037 (2)	0.030 (3)	0.041 (3)	−0.007 (2)	−0.012 (2)	0.001 (2)
C22	0.041 (3)	0.045 (3)	0.044 (3)	−0.003 (2)	−0.008 (2)	−0.004 (3)
C23	0.054 (3)	0.060 (4)	0.036 (3)	−0.010 (3)	−0.009 (2)	0.002 (3)
C24	0.047 (3)	0.060 (4)	0.047 (4)	−0.009 (3)	−0.018 (2)	0.011 (3)
C25	0.038 (3)	0.051 (3)	0.059 (4)	0.001 (2)	−0.007 (3)	0.016 (3)
C26	0.039 (2)	0.040 (3)	0.041 (3)	−0.001 (2)	−0.003 (2)	0.003 (2)

Geometric parameters (Å, º)

N1—C8	1.385 (6)	C14—H14	0.9300
N1—C2	1.404 (5)	C15—O18	1.364 (5)
N1—C12	1.455 (5)	C15—C16	1.387 (6)
C2—N3	1.289 (5)	C16—C17	1.379 (6)
C2—C19	1.459 (6)	C16—H16	0.9300
N3—C9	1.385 (5)	C17—H17	0.9300
C4—C5	1.368 (7)	O18—H18	0.8200
C4—C9	1.398 (6)	C19—C20	1.335 (6)
C4—H4	0.9300	C19—H19	0.9300
C5—C6	1.390 (7)	C20—C21	1.475 (6)
C5—H5	0.9300	C20—H20	0.9300
C6—C7	1.367 (7)	C21—C22	1.389 (6)

C6—H6	0.9300	C21—C26	1.390 (6)
C7—C10	1.406 (7)	C22—C23	1.379 (6)
C7—H7	0.9300	C22—H22	0.9300
C8—O11	1.241 (6)	C23—C24	1.382 (7)
C8—C10	1.436 (6)	C23—H23	0.9300
C9—C10	1.400 (6)	C24—C25	1.370 (7)
C12—C17	1.378 (6)	C24—H24	0.9300
C12—C13	1.381 (6)	C25—C26	1.378 (7)
C13—C14	1.377 (6)	C25—H25	0.9300
C13—H13	0.9300	C26—H26	0.9300
C14—C15	1.383 (6)		

C8—N1—C2	121.5 (4)	C15—C14—H14	119.9
C8—N1—C12	116.7 (4)	O18—C15—C14	117.4 (4)
C2—N1—C12	121.8 (3)	O18—C15—C16	123.0 (4)
N3—C2—N1	123.3 (4)	C14—C15—C16	119.6 (4)
N3—C2—C19	119.4 (4)	C17—C16—C15	120.1 (4)
N1—C2—C19	117.3 (4)	C17—C16—H16	119.9
C2—N3—C9	118.6 (4)	C15—C16—H16	119.9
C5—C4—C9	120.6 (5)	C12—C17—C16	120.0 (4)
C5—C4—H4	119.7	C12—C17—H17	120.0
C9—C4—H4	119.7	C16—C17—H17	120.0
C4—C5—C6	120.6 (5)	C15—O18—H18	109.5
C4—C5—H5	119.7	C20—C19—C2	121.6 (4)
C6—C5—H5	119.7	C20—C19—H19	119.2
C7—C6—C5	120.2 (5)	C2—C19—H19	119.2
C7—C6—H6	119.9	C19—C20—C21	126.5 (4)
C5—C6—H6	119.9	C19—C20—H20	116.8
C6—C7—C10	120.1 (5)	C21—C20—H20	116.8
C6—C7—H7	119.9	C22—C21—C26	118.3 (4)
C10—C7—H7	119.9	C22—C21—C20	123.1 (4)
O11—C8—N1	119.7 (5)	C26—C21—C20	118.7 (4)
O11—C8—C10	124.9 (5)	C23—C22—C21	120.6 (5)
N1—C8—C10	115.5 (4)	C23—C22—H22	119.7
N3—C9—C4	119.4 (4)	C21—C22—H22	119.7
N3—C9—C10	121.7 (4)	C22—C23—C24	120.3 (5)
C4—C9—C10	118.9 (4)	C22—C23—H23	119.9
C9—C10—C7	119.7 (4)	C24—C23—H23	119.9
C9—C10—C8	119.5 (4)	C25—C24—C23	119.6 (5)
C7—C10—C8	120.7 (5)	C25—C24—H24	120.2
C17—C12—C13	120.1 (4)	C23—C24—H24	120.2
C17—C12—N1	120.4 (4)	C24—C25—C26	120.4 (5)
C13—C12—N1	119.3 (4)	C24—C25—H25	119.8
C14—C13—C12	120.1 (4)	C26—C25—H25	119.8
C14—C13—H13	120.0	C25—C26—C21	120.8 (5)
C12—C13—H13	120.0	C25—C26—H26	119.6
C13—C14—C15	120.1 (4)	C21—C26—H26	119.6
C13—C14—H14	119.9		

C8—N1—C2—N3	1.2 (7)	C8—N1—C12—C17	−95.4 (5)
C12—N1—C2—N3	−177.5 (4)	C2—N1—C12—C17	83.3 (5)
C8—N1—C2—C19	−176.7 (4)	C8—N1—C12—C13	80.1 (5)
C12—N1—C2—C19	4.7 (6)	C2—N1—C12—C13	−101.2 (5)
N1—C2—N3—C9	−0.6 (6)	C17—C12—C13—C14	−0.3 (6)
C19—C2—N3—C9	177.1 (4)	N1—C12—C13—C14	−175.8 (4)
C9—C4—C5—C6	0.2 (8)	C12—C13—C14—C15	1.1 (7)
C4—C5—C6—C7	0.2 (9)	C13—C14—C15—O18	178.2 (4)
C5—C6—C7—C10	−0.3 (9)	C13—C14—C15—C16	−1.8 (7)
C2—N1—C8—O11	179.4 (5)	O18—C15—C16—C17	−178.4 (4)
C12—N1—C8—O11	−1.9 (7)	C14—C15—C16—C17	1.6 (7)
C2—N1—C8—C10	−0.7 (6)	C13—C12—C17—C16	0.1 (6)
C12—N1—C8—C10	178.0 (4)	N1—C12—C17—C16	175.5 (4)
C2—N3—C9—C4	−178.7 (4)	C15—C16—C17—C12	−0.7 (7)
C2—N3—C9—C10	−0.3 (6)	N3—C2—C19—C20	17.8 (7)
C5—C4—C9—N3	178.0 (4)	N1—C2—C19—C20	−164.3 (4)
C5—C4—C9—C10	−0.5 (7)	C2—C19—C20—C21	−175.8 (4)
N3—C9—C10—C7	−178.0 (5)	C19—C20—C21—C22	6.9 (7)
C4—C9—C10—C7	0.4 (7)	C19—C20—C21—C26	−174.5 (4)
N3—C9—C10—C8	0.7 (7)	C26—C21—C22—C23	0.4 (7)
C4—C9—C10—C8	179.1 (4)	C20—C21—C22—C23	179.0 (4)
C6—C7—C10—C9	0.0 (8)	C21—C22—C23—C24	0.5 (7)
C6—C7—C10—C8	−178.7 (5)	C22—C23—C24—C25	−1.0 (7)
O11—C8—C10—C9	179.8 (5)	C23—C24—C25—C26	0.6 (8)
N1—C8—C10—C9	−0.2 (6)	C24—C25—C26—C21	0.3 (7)
O11—C8—C10—C7	−1.6 (8)	C22—C21—C26—C25	−0.8 (7)
N1—C8—C10—C7	178.5 (5)	C20—C21—C26—C25	−179.5 (4)

Hydrogen-bond geometry (Å, º)

Cg3 and Cg4 are the centroids of the C12–C17 and C21–C26 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O18—H18···O11^{i}	0.82	1.84	2.654 (5)	172
C4—H4···*Cg*4^{ii}	0.94	2.96	3.829 (5)	157
C16—H16···*Cg*3^{i}	0.94	2.95	3.646 (5)	133

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