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2-{(*E*)-[(4-Anilinophenyl)imino]methyl}-4-[(*E*)-(4-methoxyphenyl)diazenyl]phenol

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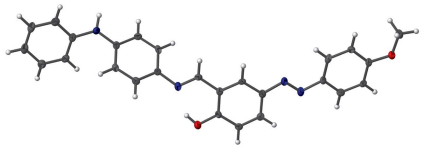
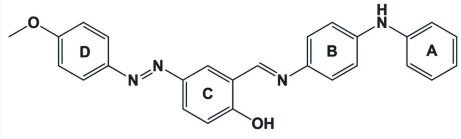
Structural data: full structural data are available from iucrdata.iucr.org

In the title Schiff base compound, $C_{26}H_{22}N_4O_2$, the hydroxy group forms a intramolecular hydrogen bond to the imine N atom and generates an *S*(6) ring motif. The conformation about the C=N and N=N bonds is *E*. The 4-methoxybenzene ring and the *p*-phenylenediamine ring are inclined to the phenol ring by 11.61 (17) and 46.04 (17)°, respectively. The terminal *N*-phenyl ring is inclined to the *p*-phenylenediamine ring by 50.72 (17)°. In the crystal, adjacent molecules are linked by C—H···O hydrogen bonds, involving the *p*-phenylenediamine ring and the phenol ring, forming chains along [001]. The chains are linked by a number of C—H···π interactions, forming slabs propagating parallel to (100).

3D view



Chemical scheme



Structure description

Azo compounds have received much attention in fundamental and applied chemistry (Nishihara, 2004; Ispir, 2009). The well known applications of azo dyes in acid–base indicators and chemical sensors and as electron-transfer catalysts have attracted the interest of many investigators (Tunçel & Serin, 2006). The versatile applications of azo compounds in various fields include dyeing textile fibres, colouring different materials, plastics, biological medical studies, lasers, liquid crystalline displays, electro-optical devices and ink-jet printers in high-technology areas (Gregory, 1991). The conversion from the *trans* to the *cis* form in azo compounds can lead to photochromism. Photochromic compounds are of great interest for the control and measurement of radiation intensity, optical computers and display systems (Dürr & Bouas-Laurent, 1990), and for potential applications in molecular electronic devices (Martin *et al.*, 1995). Schiff bases often exhibit various biological activities including antibacterial, anticancer, anti-

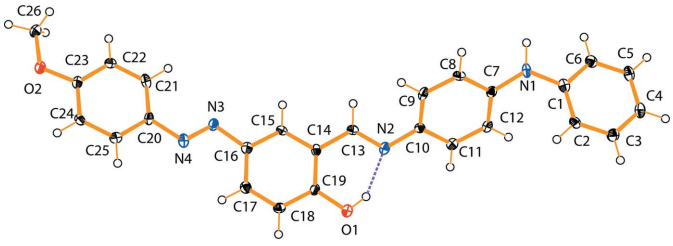


Figure 1
The molecular structure of the title compound, showing the atom labelling. Displacement ellipsoids are drawn at the 40% probability level. The intramolecular O—H···N hydrogen bond (see Table 1) is shown as a dashed line.

inflammatory and antitoxic properties (Lozier *et al.*, 1975). 2-Hydroxy salicylaldimine compounds can undergo enol–imine/keto–amine tautomerization by H-atom transfer from the hydroxyl oxygen to the imine nitrogen, probably *via* intramolecular hydrogen bonding (Khedr *et al.*, 2005). The present work is part of an ongoing structural study of Schiff bases and their utilization in the synthesis of new organic and polynuclear coordination compounds (Faizi & Hussain, 2014; Faizi *et al.*, 2016). We report herein, on the synthesis and crystal structure of a new Schiff base compound.

There are very few examples of similar compounds in the literature although some metal complexes of similar ligands have been reported (Khandar & Rezvani, 1998; Cariati *et al.* 2004). One very similar compound, used as a chemosensor for the detection of fluoride and cyanide ions, has been described (Udhayakumari *et al.* 2015), but no crystal structure has been reported. Similar azo Schiff base compounds have been synthesized and used for second-order non-linearity (Jalali-Heravi *et al.* 1999), and for non-linear optical properties (Qian, *et al.* 2004). Azo-azomethine compounds have been synthesized and used as fluorescent dyes and for the synthesis of Co^{II} and Cu^{II} complexes (Kurtoglu *et al.* 2014).

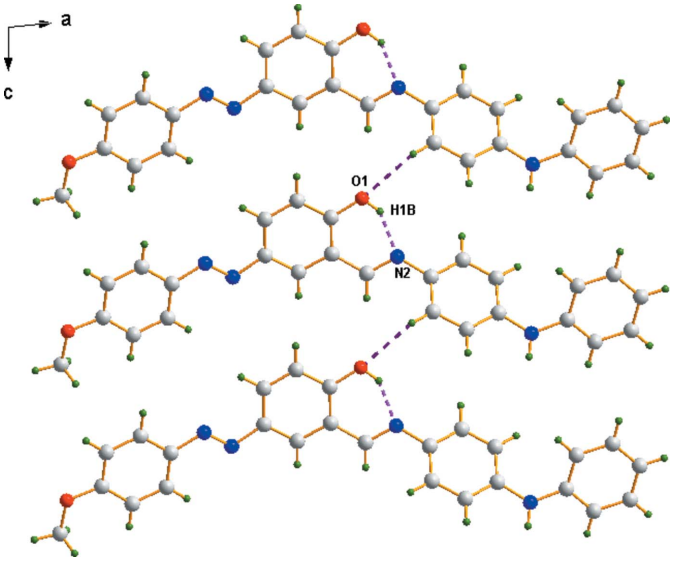


Figure 2
A view along the *b* axis of the C—H···O hydrogen-bonded chain in the crystal of the title compound. The hydrogen bonds are shown as dashed lines; see Table 1 for details).

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

*Cg*1, *Cg*2, *Cg*3 and *Cg*4 are the centroids of rings *A* (C1–C6), *B* (C7–C12), *C* (C14–C19) and *D* (C20–C25), respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*B*···N2	0.84	1.81	2.559 (4)	147
C9—H9···O1^{i}	0.95	2.45	3.307 (5)	150
C3—H3···*Cg*1^{ii}	0.95	2.83	3.509 (4)	129
C6—H6···*Cg*1^{iii}	0.95	2.87	3.556 (4)	130
C8—H8···*Cg*2^{iv}	0.95	2.80	3.538 (4)	135
C11—H11···*Cg*2^{v}	0.95	2.73	3.441 (4)	132
C15—H15···*Cg*3^{iii}	0.95	2.89	3.584 (4)	131
C18—H18···*Cg*3^{ii}	0.95	2.80	3.474 (4)	129
C22—H22···*Cg*4^{iii}	0.95	2.79	3.536 (4)	136
C25—H25···*Cg*4^{ii}	0.95	2.60	3.373 (4)	138

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

The molecular structure of the title compound is illustrated in Fig. 1. The conformation about the azomethine N2═C13 bond [1.286 (4) Å] is *E*, and the C10—N2—C13—C14 torsion angle is 170.3 (3). The molecule is non-planar, with ring *B* (C7–C12) being inclined to rings *A* (C1–C6), *C* (C14–C19) and *D* (C20–C25) by 50.72 (17), 46.04 (17) and 52.12 (17)°, respectively, while the dihedral angles *A*/*C*, *A*/*D* and *C*/*D* are 8.15 (17), 3.56 (17) and 11.61 (17)°, respectively. The N3—C16 and N4—C20 bond lengths of 1.426 (5) and 1.424 (5) Å, respectively, indicate single-bond character, whereas the N3═N4 bond length of 1.252 (4) Å confirms the double-bond character, with an *E* conformation about the N3═N4 bond.

Depending on the tautomers, two types of intramolecular hydrogen bonds are observed in Schiff bases: O—H···N in phenol–imine and N—H···O in keto–amine tautomers. The present analysis shows that the title compound exists in the phenol–imine form (Fig. 1). It exhibits an intramolecular O—H···N hydrogen bond, which generates an *S*(6) ring motif (Fig. 1 and Table 1). This intramolecular O—H···N hydrogen bond has been detected previously in salicylaldehyde derivatives (Faizi *et al.*, 2017). The C19—O1 [1.347 (4) Å] bond length is in agreement with the values reported for similar compounds, *viz*. (*E*)-2-{[(4-anilinophenyl)- imino]methyl}phenol (Faizi *et al.*, 2015).

In the crystal, molecules are connected by C—H···O hydrogen bonds, generating chains extending along the *c*-axis direction; Table 1 and Fig. 2. The chains are linked *via* a

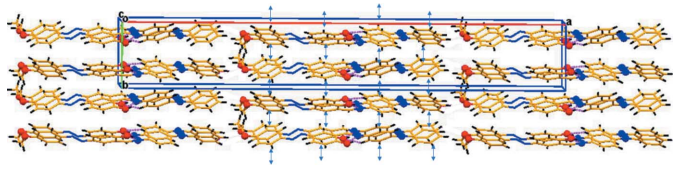


Figure 3
A view along the *c* axis of the crystal packing of the title compound. The C—H···π interactions (see Table 1) are indicated by the double-headed blue arrows.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{26}H_{22}N_4O_2$
M_r	422.47
Crystal system, space group	Monoclinic, *Cc*
Temperature (K)	100
a, *b*, *c* (Å)	47.514 (8), 7.1015 (11), 6.1289 (10)
β (°)	96.037 (9)
V (Å^3)	2056.6 (6)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.20 × 0.15 × 0.10
Data collection	
Diffractometer	Bruker *SMART APEX* CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2003)
T_{min}, T_{max}	0.953, 0.981
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11961, 3631, 2747
R_{int}	0.062
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.596
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.043, 0.092, 1.01
No. of reflections	3631
No. of parameters	292
No. of restraints	2
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.20, −0.21

Computer programs: *SMART* and *SAINT* (Bruker, 2003), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*) and *DIAMOND* (Brandenberg & Putz, 2006).

number of C—H$\cdots\pi$ interactions, forming slabs lying parallel to the *bc* plane; see Table 1 and Fig. 3.

Synthesis and crystallization

Synthesis of 5-(4-methoxyphenylazo)salicyaldehyde (*L*): To a solution of *p*-methoxyaniline in water (5 ml, 0.05 mol) 6 ml of 37% aq. HCl was slowly added at 0–5° C with stirring. 20 ml of 20% aq. $NaNO_2$ solution was added to the mixture and the resulting solution was stirred for 1 h, which gave a bright-yellow solution. Salicylaldehyde (5 ml, 0.05 mol) was dissolved in a solution comprising 18 g Na_2CO_3 and 150 ml H_2O and the resulting solution was added dropwise to the bright-yellow solution over a period of 1 h. After stirring for 4 h, the reaction mixture was neutralized with HCl, yielding a brown crude solid that was filtered and recrystallized from ethanol to afford a pure yellow product.

Synthesis of the title compound: 100 mg (1 mmol) of *N*-phenyl-*p*-phenylenediamine were dissolved in 10 ml of absolute ethanol. To this solution, 52 mg (1 mmol) of (***L***) in 5 ml of absolute ethanol was added dropwise under stirring. The mixture was stirred for 10 min, two drops of glacial acetic acid were then added and the mixture was refluxed for a further 2 h. The resulting light-brown precipitate was recovered by filtration, washed several times with small portions of EtOH and then with diethyl ether to give the title compound (yield 120 mg, 86%). Yellow needle-like crystals of the title compound were obtained within 3 d by slow evaporation of a solution in MeOH.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x170548 [https://doi.org/10.1107/S241431461700548X]

2-{(*E*)-[(4-Anilinophenyl)imino]methyl}-4-[(*E*)-(4-methoxyphenyl)-diazenyl]phenol

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Crystal data

$C_{26}H_{22}N_4O_2$
M_r = 422.47
Monoclinic, *Cc*
a = 47.514 (8) Å
b = 7.1015 (11) Å
c = 6.1289 (10) Å
β = 96.037 (9)°
V = 2056.6 (6) Å^3
Z = 4
F(000) = 888
D_x = 1.361 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 3571 reflections
θ = 2.9–24.3°
μ = 0.09 mm^{-1}
T = 100 K
Needle, yellow
0.20 × 0.15 × 0.10 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
/w–scans
Absorption correction: multi-scan (SADABS; Bruker, 2003)
T_{min} = 0.953, T_{max} = 0.981
11961 measured reflections
3631 independent reflections
2747 reflections with $I > 2\sigma(I)$
R_{int} = 0.062
θ_{max} = 25.1°, θ_{min} = 2.9°
h = −56→56
k = −8→8
l = −7→7

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.092
S = 1.01
3631 reflections
292 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0395P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Extinction correction: (SHELXL2016; Sheldrick, 2015b), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0034 (6)

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}
O2	0.28294 (6)	0.2453 (3)	0.6349 (4)	0.0227 (7)
O1	0.50798 (5)	0.1833 (4)	0.0205 (4)	0.0264 (7)
H1B	0.522153	0.205011	0.110889	0.040*
N2	0.53540 (7)	0.2769 (4)	0.3861 (5)	0.0198 (8)
N3	0.40918 (6)	0.2985 (4)	0.4118 (5)	0.0212 (8)
N4	0.38790 (6)	0.2203 (4)	0.3130 (5)	0.0218 (8)
N1	0.63876 (6)	0.2375 (4)	0.9183 (6)	0.0233 (8)
H1A	0.637112	0.227085	1.059477	0.028*
C23	0.30982 (8)	0.2495 (5)	0.5727 (6)	0.0189 (9)
C10	0.56120 (8)	0.2689 (5)	0.5255 (6)	0.0174 (9)
C14	0.48504 (8)	0.2851 (5)	0.3316 (7)	0.0177 (9)
C24	0.31294 (8)	0.1601 (5)	0.3748 (6)	0.0178 (9)
H24	0.297072	0.102594	0.293763	0.021*
C1	0.66649 (8)	0.2465 (5)	0.8587 (7)	0.0202 (10)
C16	0.43388 (8)	0.2748 (5)	0.3011 (7)	0.0194 (9)
C22	0.33303 (7)	0.3314 (5)	0.6933 (6)	0.0189 (9)
H22	0.330948	0.391784	0.828941	0.023*
C8	0.58894 (8)	0.1733 (5)	0.8577 (7)	0.0204 (9)
H8	0.590094	0.115840	0.998308	0.025*
C18	0.45831 (8)	0.1758 (5)	−0.0035 (7)	0.0198 (10)
H18	0.457845	0.129159	−0.149129	0.024*
C25	0.33910 (8)	0.1549 (5)	0.2963 (6)	0.0202 (10)
H25	0.341187	0.094179	0.160816	0.024*
C12	0.61148 (8)	0.3222 (5)	0.5708 (6)	0.0192 (9)
H12	0.628009	0.369191	0.514943	0.023*
C11	0.58566 (7)	0.3329 (5)	0.4447 (6)	0.0199 (9)
H11	0.584655	0.384689	0.301109	0.024*
C19	0.48417 (7)	0.2153 (5)	0.1163 (6)	0.0184 (10)
C2	0.67385 (8)	0.1688 (5)	0.6654 (6)	0.0203 (9)
H2	0.659660	0.114073	0.564225	0.024*
C7	0.61336 (8)	0.2431 (5)	0.7787 (6)	0.0188 (9)
C9	0.56306 (8)	0.1873 (5)	0.7325 (7)	0.0206 (9)
H9	0.546485	0.140993	0.788315	0.025*
C21	0.35935 (8)	0.3240 (5)	0.6135 (7)	0.0217 (10)
H21	0.375353	0.378276	0.696228	0.026*
C20	0.36240 (8)	0.2382 (5)	0.4144 (6)	0.0183 (10)
C3	0.70172 (8)	0.1701 (5)	0.6184 (7)	0.0240 (10)
H3	0.706527	0.117276	0.484792	0.029*
C13	0.51190 (8)	0.3059 (5)	0.4672 (7)	0.0180 (9)

H13	0.512070	0.341299	0.616818	0.022*
C6	0.68741 (8)	0.3266 (5)	1.0056 (6)	0.0231 (10)
H6	0.682584	0.381772	1.137828	0.028*
C15	0.45950 (7)	0.3168 (5)	0.4183 (6)	0.0175 (9)
H15	0.459738	0.368589	0.561428	0.021*
C17	0.43349 (9)	0.2041 (5)	0.0877 (7)	0.0210 (10)
H17	0.415930	0.175520	0.005503	0.025*
C26	0.27780 (9)	0.3453 (5)	0.8274 (7)	0.0298 (10)
H26A	0.289393	0.291821	0.954070	0.045*
H26B	0.257743	0.334788	0.849766	0.045*
H26C	0.282725	0.478167	0.811095	0.045*
C5	0.71541 (8)	0.3256 (5)	0.9584 (7)	0.0252 (10)
H5	0.729705	0.378741	1.060064	0.030*
C4	0.72263 (8)	0.2483 (5)	0.7655 (7)	0.0260 (10)
H4	0.741771	0.248696	0.733733	0.031*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O2	0.0167 (15)	0.0279 (16)	0.0236 (17)	−0.0008 (12)	0.0037 (12)	−0.0043 (13)
O1	0.0178 (16)	0.0369 (17)	0.0247 (17)	−0.0002 (13)	0.0039 (13)	−0.0030 (13)
N2	0.0162 (19)	0.0168 (19)	0.027 (2)	0.0002 (14)	0.0037 (16)	−0.0008 (14)
N3	0.0147 (19)	0.0253 (19)	0.024 (2)	0.0007 (14)	0.0020 (16)	0.0010 (14)
N4	0.016 (2)	0.0204 (18)	0.029 (2)	0.0003 (14)	0.0028 (16)	0.0015 (15)
N1	0.0173 (19)	0.034 (2)	0.018 (2)	0.0021 (14)	0.0000 (14)	0.0018 (15)
C23	0.015 (2)	0.017 (2)	0.025 (3)	0.0003 (16)	0.0027 (18)	0.0072 (18)
C10	0.017 (2)	0.018 (2)	0.018 (2)	0.0013 (17)	0.0019 (17)	−0.0023 (17)
C14	0.016 (2)	0.015 (2)	0.022 (3)	−0.0010 (16)	0.0020 (17)	0.0032 (17)
C24	0.017 (2)	0.018 (2)	0.018 (2)	−0.0024 (16)	−0.0021 (17)	−0.0002 (17)
C1	0.018 (2)	0.015 (2)	0.027 (3)	−0.0002 (17)	−0.0003 (19)	0.0050 (18)
C16	0.018 (2)	0.017 (2)	0.023 (2)	0.0019 (17)	0.0027 (18)	0.0045 (18)
C22	0.020 (2)	0.021 (2)	0.016 (2)	0.0012 (17)	0.0021 (18)	0.0003 (17)
C8	0.023 (2)	0.021 (2)	0.017 (2)	0.0011 (17)	0.0020 (18)	0.0018 (18)
C18	0.023 (2)	0.019 (2)	0.017 (2)	0.0013 (17)	0.0023 (19)	0.0009 (17)
C25	0.024 (2)	0.016 (2)	0.021 (2)	0.0025 (16)	0.0027 (19)	0.0005 (17)
C12	0.017 (2)	0.018 (2)	0.024 (3)	0.0010 (16)	0.0051 (17)	−0.0010 (18)
C11	0.022 (2)	0.018 (2)	0.021 (2)	0.0016 (17)	0.0042 (19)	0.0009 (17)
C19	0.016 (2)	0.021 (2)	0.019 (2)	0.0012 (17)	0.0048 (18)	0.0025 (17)
C2	0.021 (2)	0.018 (2)	0.021 (3)	0.0006 (17)	−0.0023 (18)	−0.0014 (17)
C7	0.016 (2)	0.018 (2)	0.022 (2)	0.0002 (17)	0.0023 (18)	−0.0044 (17)
C9	0.016 (2)	0.020 (2)	0.027 (3)	−0.0002 (16)	0.0077 (18)	−0.0040 (17)
C21	0.016 (2)	0.017 (2)	0.031 (3)	−0.0001 (16)	−0.0037 (18)	0.0009 (19)
C20	0.014 (2)	0.019 (2)	0.023 (3)	0.0013 (16)	0.0024 (18)	0.0000 (17)
C3	0.024 (2)	0.022 (2)	0.026 (3)	0.0062 (17)	0.0027 (19)	0.0012 (18)
C13	0.021 (2)	0.019 (2)	0.014 (2)	0.0004 (16)	0.0018 (17)	0.0015 (16)
C6	0.025 (3)	0.021 (2)	0.024 (3)	0.0073 (17)	0.0001 (19)	−0.0008 (17)
C15	0.020 (2)	0.019 (2)	0.013 (2)	0.0000 (17)	−0.0008 (17)	−0.0013 (16)
C17	0.020 (2)	0.021 (2)	0.022 (3)	−0.0017 (17)	0.0001 (18)	0.0027 (18)

C26	0.020 (2)	0.041 (3)	0.029 (3)	0.0015 (18)	0.0068 (18)	−0.006 (2)
C5	0.019 (2)	0.018 (2)	0.037 (3)	−0.0011 (16)	−0.003 (2)	0.001 (2)
C4	0.018 (2)	0.022 (2)	0.037 (3)	0.0027 (17)	0.000 (2)	0.0044 (19)

Geometric parameters (Å, º)

O2—C23	1.371 (4)	C8—H8	0.9500
O2—C26	1.420 (5)	C18—C17	1.372 (5)
O1—C19	1.347 (4)	C18—C19	1.392 (5)
O1—H1B	0.8400	C18—H18	0.9500
N2—C13	1.286 (4)	C25—C20	1.390 (5)
N2—C10	1.420 (4)	C25—H25	0.9500
N3—N4	1.252 (4)	C12—C11	1.382 (5)
N3—C16	1.426 (5)	C12—C7	1.386 (6)
N4—C20	1.424 (5)	C12—H12	0.9500
N1—C7	1.405 (5)	C11—H11	0.9500
N1—C1	1.405 (5)	C2—C3	1.385 (5)
N1—H1A	0.8800	C2—H2	0.9500
C23—C22	1.389 (5)	C9—H9	0.9500
C23—C24	1.391 (5)	C21—C20	1.385 (6)
C10—C11	1.387 (5)	C21—H21	0.9500
C10—C9	1.389 (5)	C3—C4	1.385 (6)
C14—C15	1.393 (5)	C3—H3	0.9500
C14—C19	1.406 (6)	C13—H13	0.9500
C14—C13	1.455 (5)	C6—C5	1.391 (5)
C24—C25	1.380 (5)	C6—H6	0.9500
C24—H24	0.9500	C15—H15	0.9500
C1—C2	1.385 (5)	C17—H17	0.9500
C1—C6	1.390 (5)	C26—H26A	0.9800
C16—C15	1.380 (5)	C26—H26B	0.9800
C16—C17	1.399 (6)	C26—H26C	0.9800
C22—C21	1.391 (4)	C5—C4	1.379 (6)
C22—H22	0.9500	C5—H5	0.9500
C8—C9	1.383 (5)	C4—H4	0.9500
C8—C7	1.394 (5)		
C23—O2—C26	117.8 (3)	O1—C19—C14	121.7 (3)
C19—O1—H1B	109.5	C18—C19—C14	120.2 (3)
C13—N2—C10	120.3 (3)	C1—C2—C3	120.6 (4)
N4—N3—C16	112.4 (3)	C1—C2—H2	119.7
N3—N4—C20	115.5 (3)	C3—C2—H2	119.7
C7—N1—C1	127.5 (4)	C12—C7—C8	119.2 (4)
C7—N1—H1A	116.2	C12—C7—N1	122.7 (4)
C1—N1—H1A	116.2	C8—C7—N1	118.1 (4)
O2—C23—C22	124.9 (4)	C8—C9—C10	120.3 (4)
O2—C23—C24	114.9 (3)	C8—C9—H9	119.9
C22—C23—C24	120.3 (4)	C10—C9—H9	119.9
C11—C10—C9	119.2 (4)	C20—C21—C22	120.5 (4)

C11—C10—N2	118.4 (3)	C20—C21—H21	119.7
C9—C10—N2	122.3 (3)	C22—C21—H21	119.7
C15—C14—C19	118.3 (4)	C21—C20—C25	119.6 (4)
C15—C14—C13	120.8 (4)	C21—C20—N4	126.6 (3)
C19—C14—C13	120.6 (4)	C25—C20—N4	113.7 (3)
C25—C24—C23	119.9 (3)	C2—C3—C4	120.2 (4)
C25—C24—H24	120.1	C2—C3—H3	119.9
C23—C24—H24	120.1	C4—C3—H3	119.9
C2—C1—C6	119.3 (4)	N2—C13—C14	120.5 (4)
C2—C1—N1	122.2 (4)	N2—C13—H13	119.7
C6—C1—N1	118.5 (4)	C14—C13—H13	119.7
C15—C16—C17	119.3 (4)	C5—C6—C1	119.9 (4)
C15—C16—N3	116.9 (4)	C5—C6—H6	120.1
C17—C16—N3	123.8 (3)	C1—C6—H6	120.1
C23—C22—C21	119.4 (4)	C16—C15—C14	121.5 (4)
C23—C22—H22	120.3	C16—C15—H15	119.3
C21—C22—H22	120.3	C14—C15—H15	119.3
C9—C8—C7	120.4 (4)	C18—C17—C16	120.4 (4)
C9—C8—H8	119.8	C18—C17—H17	119.8
C7—C8—H8	119.8	C16—C17—H17	119.8
C17—C18—C19	120.3 (4)	O2—C26—H26A	109.5
C17—C18—H18	119.9	O2—C26—H26B	109.5
C19—C18—H18	119.9	H26A—C26—H26B	109.5
C24—C25—C20	120.3 (4)	O2—C26—H26C	109.5
C24—C25—H25	119.8	H26A—C26—H26C	109.5
C20—C25—H25	119.8	H26B—C26—H26C	109.5
C11—C12—C7	120.3 (4)	C4—C5—C6	120.6 (4)
C11—C12—H12	119.9	C4—C5—H5	119.7
C7—C12—H12	119.9	C6—C5—H5	119.7
C12—C11—C10	120.6 (4)	C5—C4—C3	119.5 (4)
C12—C11—H11	119.7	C5—C4—H4	120.3
C10—C11—H11	119.7	C3—C4—H4	120.3
O1—C19—C18	118.1 (4)		

C16—N3—N4—C20	180.0 (3)	C1—N1—C7—C12	−23.0 (6)
C26—O2—C23—C22	5.6 (5)	C1—N1—C7—C8	159.8 (3)
C26—O2—C23—C24	−175.7 (3)	C7—C8—C9—C10	0.8 (6)
C13—N2—C10—C11	−147.4 (3)	C11—C10—C9—C8	1.1 (6)
C13—N2—C10—C9	37.3 (6)	N2—C10—C9—C8	176.4 (4)
O2—C23—C24—C25	−179.8 (3)	C23—C22—C21—C20	0.8 (5)
C22—C23—C24—C25	−0.9 (6)	C22—C21—C20—C25	−1.6 (6)
C7—N1—C1—C2	−34.1 (6)	C22—C21—C20—N4	180.0 (3)
C7—N1—C1—C6	149.8 (4)	C24—C25—C20—C21	1.0 (5)
N4—N3—C16—C15	−165.6 (3)	C24—C25—C20—N4	179.7 (3)
N4—N3—C16—C17	11.3 (5)	N3—N4—C20—C21	−3.5 (5)
O2—C23—C22—C21	179.1 (3)	N3—N4—C20—C25	178.0 (3)
C24—C23—C22—C21	0.4 (5)	C1—C2—C3—C4	0.5 (5)
C23—C24—C25—C20	0.2 (5)	C10—N2—C13—C14	−170.3 (3)

C7—C12—C11—C10	1.5 (5)	C15—C14—C13—N2	−179.8 (3)
C9—C10—C11—C12	−2.3 (5)	C19—C14—C13—N2	6.2 (6)
N2—C10—C11—C12	−177.7 (3)	C2—C1—C6—C5	−0.8 (5)
C17—C18—C19—O1	179.3 (3)	N1—C1—C6—C5	175.4 (3)
C17—C18—C19—C14	−0.2 (5)	C17—C16—C15—C14	−2.0 (6)
C15—C14—C19—O1	179.2 (3)	N3—C16—C15—C14	175.1 (3)
C13—C14—C19—O1	−6.7 (5)	C19—C14—C15—C16	2.5 (5)
C15—C14—C19—C18	−1.3 (5)	C13—C14—C15—C16	−171.6 (3)
C13—C14—C19—C18	172.8 (4)	C19—C18—C17—C16	0.7 (5)
C6—C1—C2—C3	0.1 (5)	C15—C16—C17—C18	0.4 (5)
N1—C1—C2—C3	−176.0 (3)	N3—C16—C17—C18	−176.5 (3)
C11—C12—C7—C8	0.5 (5)	C1—C6—C5—C4	0.9 (5)
C11—C12—C7—N1	−176.6 (3)	C6—C5—C4—C3	−0.4 (6)
C9—C8—C7—C12	−1.7 (6)	C2—C3—C4—C5	−0.4 (6)
C9—C8—C7—N1	175.6 (3)		

Hydrogen-bond geometry (Å, º)

Cg1, Cg2, Cg3 and Cg4 are the centroids of rings *A* (C1–C6), *B* (C7–C12), *C* (C14–C19) and *D* (C20–C25), respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*B*···N2	0.84	1.81	2.559 (4)	147
C9—H9···O1^{i}	0.95	2.45	3.307 (5)	150
C3—H3···*Cg*1^{ii}	0.95	2.83	3.509 (4)	129
C6—H6···*Cg*1^{iii}	0.95	2.87	3.556 (4)	130
C8—H8···*Cg*2^{iv}	0.95	2.80	3.538 (4)	135
C11—H11···*Cg*2^{v}	0.95	2.73	3.441 (4)	132
C15—H15···*Cg*3^{iii}	0.95	2.89	3.584 (4)	131
C18—H18···*Cg*3^{ii}	0.95	2.80	3.474 (4)	129
C22—H22···*Cg*4^{iii}	0.95	2.79	3.536 (4)	136
C25—H25···*Cg*4^{ii}	0.95	2.60	3.373 (4)	138

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