CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

Received 21 November 2014
Accepted 1 December 2014

Edited by H. Stoeckli-Evans, University of Neuchâtel, Switzerland

Keywords: crystal structure; Schiff base; azines; dimers; C—H···π contacts

CCDC reference: 1036846
Supporting information: this article has supporting information at journals.iucr.org/e

Crystal structure of (*Z*)-2-[(*E*)-2-benzylidenehydrazin-1-ylidene]-1,2-diphenylethanone

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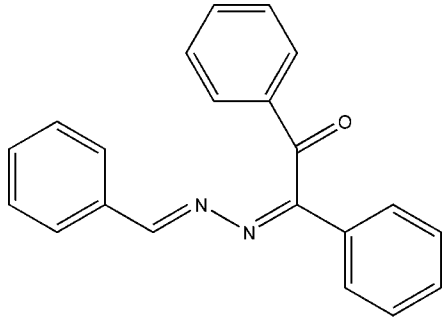
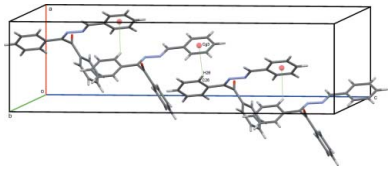
The title compound, $C_{21}H_{16}N_2O$, has an almost planar (r.m.s. deviation = 0.0074 Å) 1,2-dibenzylidenehydrazine backbone with an approximately orthogonal almost planar (r.m.s. deviation = 0.0368 Å) phenylethanone substituent on one of the imine C atoms. The dihedral angle between the two mean planes is 76.99 (4)°. In the crystal, molecules are linked *via* C—H···O hydrogen bonds and C—H···π contacts, forming a three-dimensional structure with molecules stacked along the *a*-axis direction.

1. Chemical context

Aromatic carbonyl compounds react easily with hydrazines to form hydrazones, which can condense with a second molecule of a carbonyl compound to yield an azine. As a result of their fascinating physical and chemical properties, azines and their derivatives have been utilized extensively in areas such as dyes (Kim *et al.*, 2010) and non-linear fluorophores (Facchetti *et al.*, 2002). They are also noted for their biological and pharmaceutical applications (Wadher *et al.*, 2009; Pandeya *et al.*, 1999). Furthermore, there are many reports of polyazines as highly conjugated polymers functioning in electronic, optoelectronic and photonic applications (Dudis *et al.*, 1993). As part of our studies of Schiff base azines, the title compound was synthesized and its molecular and crystal structure are reported on herein.





2. Structural commentary

The molecule of the title compound, Fig. 1, comprises a 1,2-dibenzylidenehydrazine backbone with a phenyl ethanone substituent on atom C2. Both the hydrazine and ethanone fragments are approximately planar with r.m.s. deviations of 0.0074 Å from the O1/C1/C11–C16 mean plane and 0.0368 Å from the plane through the 16 atoms of the dibenzyl-

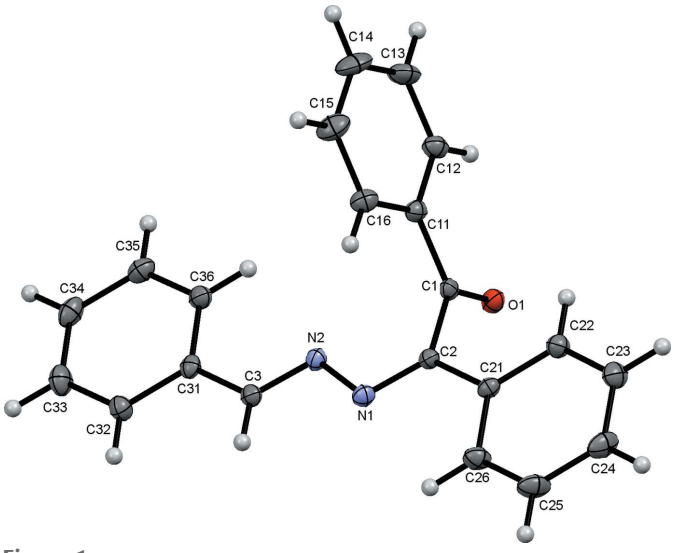


Figure 1
The molecular structure of the title compound, showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

idenehydrazine unit. The two mean planes are almost orthogonal with a dihedral angle of 76.99 (4)°. The molecule adopts a *Z* conformation with respect to the C2═N1 bond and an *E* conformation with respect to the C3═N2 bond, with the carbonyl atom O1 and the C11–C16 phenyl ring located on opposite sides of the dibenzylidenehydrazine plane. The bond lengths and angles in the title molecule agree reasonably well with those found in closely related structures (Abbasi *et al.*, 2007; Wieland *et al.*, 2011).

3. Supramolecular features

In the crystal, a pair of C35—H35···O1 hydrogen bonds link adjacent molecules into dimers with $R_2^2(20)$ ring motifs (Fig. 2 and Table 1). Atom O1 is also involved in two further C—H···O hydrogen bonds, C3—H3···O1 and C32—H32···O1 that generate $R_2^1(6)$ ring motifs. These contacts link the dimers into stacks parallel to (011); see Table 1 and Fig. 2. Interestingly, neither of the hydrazine N atoms are involved in significantly close intermolecular contacts with the shortest intermolecular H12···N1 contact being *ca* 2.85 Å. A contribution to the packing is, however, made by a C—H···π

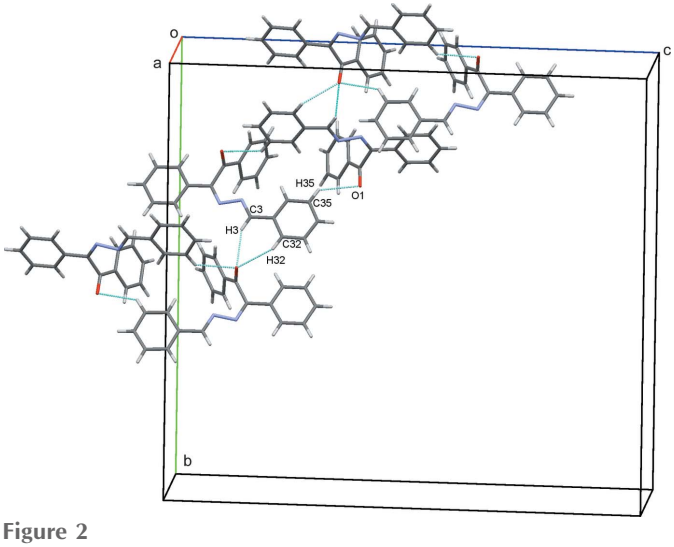


Figure 2
A view of the dimers formed *via* C—H···O contacts (blue dashed lines; see Table 1 for details) and linked into stacks running parallel to (011) in the crystal of the title compound.

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

Cg is the centroid of the C31–C36 phenyl ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C35—H35···O1^{i}	0.95	2.61	3.337 (3)	134
C3—H3···O1^{ii}	0.95	2.41	3.272 (3)	151
C32—H32···O1^{ii}	0.95	2.68	3.478 (3)	141
C26—H26···*Cg*^{iii}	0.95	2.97	3.699 (3)	135

Symmetry codes: (i) $x, -y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x+\frac{1}{4}, y-\frac{1}{4}, -z+\frac{3}{4}$; (iii) $x+\frac{1}{4}, -y+\frac{1}{4}, z+\frac{1}{4}$.

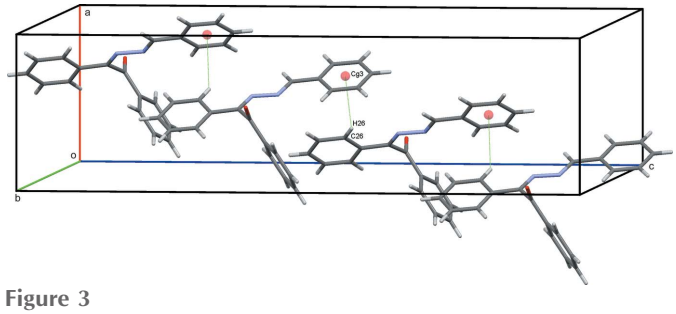


Figure 3
A view of the chains along the *c*-axis direction formed by C—H···π contacts in the crystal of the title compound (shown as green dotted lines with the ring centroids displayed as coloured spheres, see Table 1 for details).

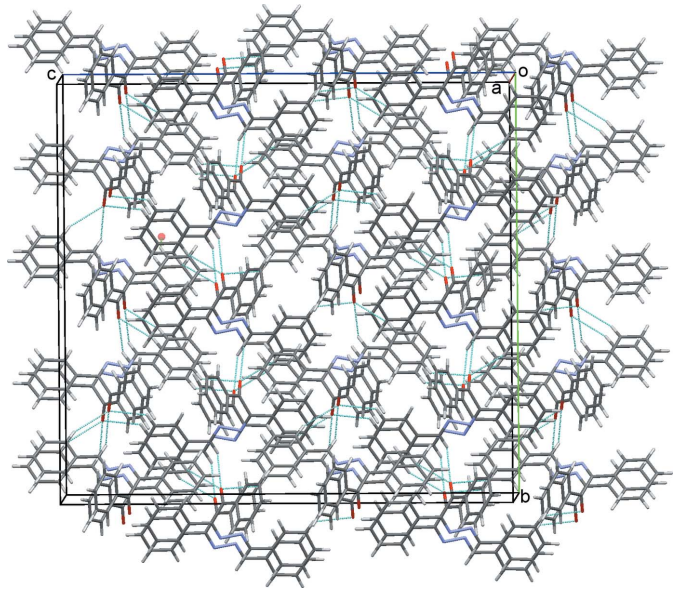


Figure 4
A view along the *a*-axis direction of the crystal packing of the title compound. Hydrogen bonds are drawn as blue dashed lines with a representative C—H···π contact shown as a green dotted line (see Table 1 for details).

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{21}H_{16}N_2O$
M_r	312.36
Crystal system, space group	Orthorhombic, *F*2*dd*
Temperature (K)	150
a, *b*, *c* (Å)	8.1653 (3), 27.6113 (11), 29.6818 (13)
V (Å^3)	6691.9 (5)
Z	16
Radiation type	Mo *Kα*
μ (mm^{-1})	0.08
Crystal size (mm)	0.55 × 0.29 × 0.24
Data collection	
Diffractometer	Bruker APEXII
Absorption correction	Multi-scan (*SADABS*; Bruker, 2006)
T_{min}, T_{max}	0.884, 0.982
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8049, 3350, 3036
R_{int}	0.032
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.649
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.039, 0.094, 1.06
No. of reflections	3350
No. of parameters	217
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.18, −0.16

Computer programs: *APEX2* and *SAINT* (Bruker, 2006), *SIR97* (Altomare *et al.*, 1999), *SHELXL2014* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2008), *CRYSCAL* (T. Roisnel, local program), *enCIFer* (Allen *et al.*, 2004), *PLATON* (Spek, 2009), *WinGX* (Farrugia, 2012) and *publCIF* (Westrip 2010).

interaction (Table 1). These interactions link molecules in a head-to-tail fashion, forming chains along *c*, as shown in Fig. 3. With 16 molecules in the orthorhombic unit cell, these various contacts combine to form a three dimensional structure with molecules stacked along the *a*-axis direction, as shown in Fig. 4.

4. Database survey

A search for the (benzylidenehydrazono)-1,2-diphenylethanone skeleton in the Cambridge Structural Database (Version 5.35, November 2013 with three updates; Groom & Allen, 2014) revealed only 7 similar compounds. The closest to the title structure are 2-{(*Z*)-2-[(*E*)-1-(2-hydroxyphenyl)methylidene]hydrazono}-1,2-diphenylethan-1-one (Abbasi *et al.*, 2007), with an hydroxy substituent in the *p* position on the equivalent of the benzene ring, and 1,2-diphenyl-2-[4-(4-pyridyl)benzylidenehydrazono]ethan-1-one, with a pyridyl ring in the same position (Patra & Ng, 2009). Two reports of polymorphs of the symmetrical 2,2′-(1,2-hydrazinediylidene)-bis(diphenylethanone) have also appeared (Patra *et al.*, 2009; Wieland *et al.*, 2011)

5. Synthesis and crystallization

A mixture of benzaldehyde (0.01 mol, 1.06 g), benzil (0.01 mol, 2.10 g) and hydrazine hydrate (0.01 mol, 0.32 g) in 50 ml of ethanol containing 2 drops of acetic acid was refluxed for about 2 h. The reaction was monitored by TLC until completion. Excess solvent was evaporated under vacuum and the resulting yellow solid product was recrystallized from absolute ethanol to afford yellow needles of the title compound (m.p. 453 K, 75% yield). Analysis calculated for $C_{21}H_{16}N_2O$ (312.36): C 80.75, H 5.16, N 8.97%; found: C 80.73, H 5.17, N 9.01%.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The C-bound H atoms were included in calculated positions and treated as riding atoms: C—H = 0.95 Å with $U_{iso} = 1.2U_{eq}$(C).

Acknowledgements

The authors acknowledge the Algerian Ministry of Higher Education and Scientific Research, the Algerian Directorate General for Scientific Research and Technological Development, and Ferhat Abbas Sétif 1 University for financial support. The Chemistry Department of the University of Otago is also thanked for support of the work of JS. Dr Lahcène Ouahab from the University of Rennes 1, France, is thanked for the data collection.

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supporting information

Acta Cryst. (2015). E**71**, 35-37 [doi:10.1107/S2056989014026358]

Crystal structure of (*Z*)-2-[(*E*)-2-benzylidenehydrazin-1-ylidene]-1,2-diphenylethanone

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Computing details

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT* (Bruker, 2006); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *CRYSCAL* (T. Roisnel, local program), *SHELXL2014* (Sheldrick, 2008), *enCIFer* (Allen *et al.*, 2004), *PLATON* (Spek, 2009), *publCIF* (Westrip 2010) and *WinGX* (Farrugia, 2012).

(*Z*)-2-[(*E*)-2-Benzylidenehydrazin-1-ylidene]-1,2-diphenylethanone

Crystal data

$C_{21}H_{16}N_2O$
M_r = 312.36
Orthorhombic, *F*2*dd*
Hall symbol: F -2d 2
a = 8.1653 (3) Å
b = 27.6113 (11) Å
c = 29.6818 (13) Å
V = 6691.9 (5) Å^3
Z = 16
F(000) = 2624
D_x = 1.240 Mg m^{-3}
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 2807 reflections
θ = 2.7–27.3°
μ = 0.08 mm^{-1}
T = 150 K
Prism, yellow
0.55 × 0.29 × 0.24 mm

Data collection

Bruker APEXII diffractometer
Radiation source: fine-focus sealed tube
CCD rotation images, thin slices scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2006)
T_{min} = 0.884, T_{max} = 0.982
8049 measured reflections
3350 independent reflections
3036 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 27.5°, θ_{min} = 3.0°
h = −9→10
k = −35→24
l = −38→38

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.094
S = 1.06
3350 reflections
217 parameters
1 restraint
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0407P)^2 + 4.1058P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C11	0.4692 (3)	0.24563 (8)	0.36467 (7)	0.0255 (5)
C12	0.4156 (3)	0.28709 (9)	0.34210 (7)	0.0316 (5)
H12	0.4758	0.3164	0.3444	0.038*
C13	0.2746 (3)	0.28525 (11)	0.31643 (9)	0.0426 (7)
H13	0.2381	0.3134	0.3010	0.051*
C14	0.1865 (3)	0.24267 (12)	0.31313 (10)	0.0504 (8)
H14	0.0888	0.2418	0.2958	0.060*
C15	0.2393 (4)	0.20147 (11)	0.33483 (10)	0.0453 (7)
H15	0.1790	0.1722	0.3322	0.054*
C16	0.3810 (3)	0.20282 (9)	0.36059 (8)	0.0326 (6)
H16	0.4178	0.1744	0.3755	0.039*
C1	0.6212 (3)	0.24786 (8)	0.39198 (6)	0.0222 (4)
O1	0.7037 (2)	0.28433 (5)	0.39542 (5)	0.0300 (4)
C2	0.6774 (3)	0.20274 (8)	0.41744 (7)	0.0220 (5)
C21	0.6542 (3)	0.20065 (8)	0.46670 (6)	0.0234 (5)
C22	0.5622 (3)	0.23566 (9)	0.48904 (7)	0.0291 (5)
H22	0.5110	0.2608	0.4723	0.035*
C23	0.5449 (3)	0.23409 (10)	0.53561 (8)	0.0344 (6)
H23	0.4825	0.2582	0.5507	0.041*
C24	0.6182 (3)	0.19755 (11)	0.55991 (8)	0.0401 (6)
H24	0.6067	0.1966	0.5917	0.048*
C25	0.7083 (4)	0.16228 (11)	0.53816 (8)	0.0406 (7)
H25	0.7575	0.1369	0.5550	0.049*
C26	0.7272 (3)	0.16376 (9)	0.49169 (8)	0.0332 (6)
H26	0.7901	0.1396	0.4769	0.040*
N1	0.7555 (2)	0.16872 (7)	0.39690 (6)	0.0265 (4)
N2	0.7675 (2)	0.17867 (7)	0.35026 (6)	0.0255 (4)
C3	0.8450 (3)	0.14520 (8)	0.32965 (7)	0.0245 (5)
H3	0.8903	0.1192	0.3465	0.029*
C31	0.8657 (3)	0.14596 (8)	0.28078 (7)	0.0252 (5)
C32	0.9510 (3)	0.10863 (9)	0.25997 (8)	0.0307 (5)
H32	0.9991	0.0838	0.2777	0.037*
C33	0.9664 (3)	0.10743 (10)	0.21338 (8)	0.0383 (6)
H33	1.0228	0.0814	0.1993	0.046*
C34	0.9002 (3)	0.14389 (9)	0.18749 (8)	0.0371 (6)
H34	0.9115	0.1431	0.1556	0.045*
C35	0.8166 (3)	0.18203 (10)	0.20799 (8)	0.0346 (6)
H35	0.7721	0.2074	0.1902	0.041*
C36	0.7987 (3)	0.18291 (9)	0.25427 (8)	0.0294 (5)

H36	0.7406	0.2087	0.2682	0.035*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.0250 (11)	0.0314 (12)	0.0200 (9)	0.0026 (11)	0.0015 (8)	0.0014 (8)
C12	0.0328 (13)	0.0337 (13)	0.0283 (11)	0.0066 (11)	−0.0003 (10)	0.0044 (10)
C13	0.0368 (15)	0.0525 (17)	0.0385 (14)	0.0136 (14)	−0.0061 (11)	0.0126 (12)
C14	0.0283 (15)	0.076 (2)	0.0472 (15)	−0.0018 (15)	−0.0157 (12)	0.0105 (15)
C15	0.0348 (15)	0.0542 (17)	0.0471 (15)	−0.0116 (14)	−0.0096 (12)	0.0049 (13)
C16	0.0298 (13)	0.0375 (14)	0.0304 (11)	−0.0016 (12)	−0.0019 (9)	0.0049 (10)
C1	0.0268 (11)	0.0233 (11)	0.0166 (8)	0.0035 (10)	0.0021 (8)	−0.0012 (8)
O1	0.0370 (10)	0.0233 (8)	0.0298 (8)	−0.0021 (8)	−0.0063 (7)	0.0013 (6)
C2	0.0214 (11)	0.0228 (10)	0.0217 (9)	−0.0008 (10)	−0.0023 (8)	0.0004 (8)
C21	0.0236 (12)	0.0262 (11)	0.0205 (9)	−0.0027 (9)	−0.0012 (8)	0.0029 (8)
C22	0.0292 (13)	0.0311 (13)	0.0268 (11)	0.0028 (11)	0.0008 (9)	0.0009 (9)
C23	0.0317 (14)	0.0428 (15)	0.0288 (12)	0.0041 (12)	0.0054 (10)	−0.0010 (10)
C24	0.0344 (14)	0.0655 (18)	0.0203 (10)	0.0006 (14)	0.0028 (10)	0.0063 (12)
C25	0.0372 (15)	0.0549 (17)	0.0297 (12)	0.0075 (14)	−0.0009 (10)	0.0153 (11)
C26	0.0347 (14)	0.0367 (14)	0.0284 (12)	0.0061 (12)	0.0004 (10)	0.0079 (10)
N1	0.0320 (11)	0.0263 (10)	0.0212 (9)	0.0019 (9)	−0.0025 (8)	0.0019 (7)
N2	0.0317 (11)	0.0248 (10)	0.0201 (9)	0.0012 (9)	−0.0014 (8)	−0.0013 (7)
C3	0.0258 (12)	0.0213 (11)	0.0265 (10)	−0.0013 (10)	−0.0021 (8)	0.0005 (9)
C31	0.0237 (12)	0.0250 (11)	0.0268 (10)	−0.0049 (10)	−0.0009 (9)	−0.0034 (9)
C32	0.0327 (14)	0.0296 (12)	0.0299 (12)	0.0014 (11)	0.0035 (9)	−0.0009 (9)
C33	0.0395 (16)	0.0419 (15)	0.0335 (13)	−0.0008 (13)	0.0100 (10)	−0.0070 (11)
C34	0.0386 (15)	0.0490 (16)	0.0238 (10)	−0.0104 (13)	0.0031 (10)	−0.0019 (10)
C35	0.0359 (14)	0.0378 (14)	0.0299 (12)	−0.0038 (12)	−0.0064 (10)	0.0054 (10)
C36	0.0319 (13)	0.0256 (12)	0.0307 (11)	−0.0002 (11)	−0.0049 (10)	0.0005 (9)

Geometric parameters (Å, º)

C11—C16	1.390 (3)	C23—H23	0.9500
C11—C12	1.397 (3)	C24—C25	1.381 (4)
C11—C1	1.483 (3)	C24—H24	0.9500
C12—C13	1.382 (4)	C25—C26	1.388 (3)
C12—H12	0.9500	C25—H25	0.9500
C13—C14	1.382 (4)	C26—H26	0.9500
C13—H13	0.9500	N1—N2	1.415 (2)
C14—C15	1.377 (4)	N2—C3	1.276 (3)
C14—H14	0.9500	C3—C31	1.461 (3)
C15—C16	1.387 (4)	C3—H3	0.9500
C15—H15	0.9500	C31—C32	1.389 (3)
C16—H16	0.9500	C31—C36	1.400 (3)
C1—O1	1.216 (3)	C32—C33	1.389 (3)
C1—C2	1.528 (3)	C32—H32	0.9500
C2—N1	1.288 (3)	C33—C34	1.377 (4)
C2—C21	1.476 (3)	C33—H33	0.9500

C21—C22	1.392 (3)	C34—C35	1.395 (4)
C21—C26	1.394 (3)	C34—H34	0.9500
C22—C23	1.390 (3)	C35—C36	1.382 (3)
C22—H22	0.9500	C35—H35	0.9500
C23—C24	1.377 (4)	C36—H36	0.9500

C16—C11—C12	119.5 (2)	C23—C24—C25	120.2 (2)
C16—C11—C1	121.1 (2)	C23—C24—H24	119.9
C12—C11—C1	119.4 (2)	C25—C24—H24	119.9
C13—C12—C11	119.7 (2)	C24—C25—C26	120.2 (2)
C13—C12—H12	120.1	C24—C25—H25	119.9
C11—C12—H12	120.1	C26—C25—H25	119.9
C12—C13—C14	120.3 (2)	C25—C26—C21	120.2 (2)
C12—C13—H13	119.9	C25—C26—H26	119.9
C14—C13—H13	119.9	C21—C26—H26	119.9
C15—C14—C13	120.4 (2)	C2—N1—N2	110.84 (16)
C15—C14—H14	119.8	C3—N2—N1	111.29 (17)
C13—C14—H14	119.8	N2—C3—C31	121.5 (2)
C14—C15—C16	119.8 (3)	N2—C3—H3	119.2
C14—C15—H15	120.1	C31—C3—H3	119.2
C16—C15—H15	120.1	C32—C31—C36	119.1 (2)
C15—C16—C11	120.2 (2)	C32—C31—C3	119.3 (2)
C15—C16—H16	119.9	C36—C31—C3	121.6 (2)
C11—C16—H16	119.9	C31—C32—C33	120.4 (2)
O1—C1—C11	122.96 (19)	C31—C32—H32	119.8
O1—C1—C2	117.85 (19)	C33—C32—H32	119.8
C11—C1—C2	119.19 (19)	C34—C33—C32	120.2 (2)
N1—C2—C21	120.24 (19)	C34—C33—H33	119.9
N1—C2—C1	120.61 (18)	C32—C33—H33	119.9
C21—C2—C1	118.91 (18)	C33—C34—C35	120.1 (2)
C22—C21—C26	118.99 (19)	C33—C34—H34	120.0
C22—C21—C2	120.9 (2)	C35—C34—H34	120.0
C26—C21—C2	120.1 (2)	C36—C35—C34	119.9 (2)
C23—C22—C21	120.4 (2)	C36—C35—H35	120.0
C23—C22—H22	119.8	C34—C35—H35	120.0
C21—C22—H22	119.8	C35—C36—C31	120.3 (2)
C24—C23—C22	120.0 (2)	C35—C36—H36	119.8
C24—C23—H23	120.0	C31—C36—H36	119.8
C22—C23—H23	120.0		

C16—C11—C12—C13	0.7 (3)	C2—C21—C22—C23	−178.2 (2)
C1—C11—C12—C13	179.7 (2)	C21—C22—C23—C24	−0.4 (4)
C11—C12—C13—C14	0.2 (4)	C22—C23—C24—C25	−0.3 (4)
C12—C13—C14—C15	−1.0 (4)	C23—C24—C25—C26	0.8 (4)
C13—C14—C15—C16	0.7 (5)	C24—C25—C26—C21	−0.5 (4)
C14—C15—C16—C11	0.2 (4)	C22—C21—C26—C25	−0.2 (4)
C12—C11—C16—C15	−1.0 (3)	C2—C21—C26—C25	178.7 (2)
C1—C11—C16—C15	−179.9 (2)	C21—C2—N1—N2	−178.27 (18)

C16—C11—C1—O1	178.1 (2)	C1—C2—N1—N2	−3.8 (3)
C12—C11—C1—O1	−0.8 (3)	C2—N1—N2—C3	179.9 (2)
C16—C11—C1—C2	−2.4 (3)	N1—N2—C3—C31	176.64 (19)
C12—C11—C1—C2	178.7 (2)	N2—C3—C31—C32	−180.0 (2)
O1—C1—C2—N1	−100.0 (2)	N2—C3—C31—C36	−1.3 (3)
C11—C1—C2—N1	80.6 (3)	C36—C31—C32—C33	−1.4 (4)
O1—C1—C2—C21	74.6 (3)	C3—C31—C32—C33	177.3 (2)
C11—C1—C2—C21	−104.9 (2)	C31—C32—C33—C34	1.5 (4)
N1—C2—C21—C22	−176.3 (2)	C32—C33—C34—C35	−0.4 (4)
C1—C2—C21—C22	9.1 (3)	C33—C34—C35—C36	−0.7 (4)
N1—C2—C21—C26	4.9 (3)	C34—C35—C36—C31	0.7 (4)
C1—C2—C21—C26	−169.7 (2)	C32—C31—C36—C35	0.4 (4)
C26—C21—C22—C23	0.6 (4)	C3—C31—C36—C35	−178.3 (2)

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the C31–C36 phenyl ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C35—H35···O1^{i}	0.95	2.61	3.337 (3)	134
C3—H3···O1^{ii}	0.95	2.41	3.272 (3)	151
C32—H32···O1^{ii}	0.95	2.68	3.478 (3)	141
C26—H26···*Cg*^{iii}	0.95	2.97	3.699 (3)	135

Symmetry codes: (i) *x*, −*y*+1/2, −*z*+1/2; (ii) *x*+1/4, *y*−1/4, −*z*+3/4; (iii) *x*+1/4, −*y*+1/4, *z*+1/4.