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(Z)-3-Anilino-1,3-diphenylprop-2-en-1-one

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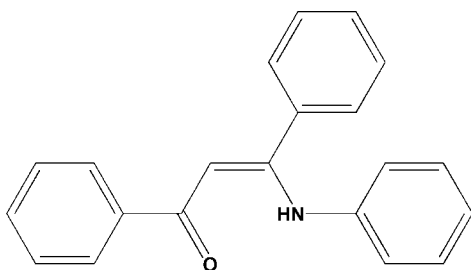
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 Key indicators: single-crystal X-ray study; $T = 294$ K; mean $\sigma(\text{C}-\text{C}) = 0.007$ Å; R factor = 0.080; wR factor = 0.249; data-to-parameter ratio = 13.3.

In the title compound, $\text{C}_{21}\text{H}_{17}\text{NO}$, the phenyl ring directly linked to the carbonyl group is oriented at an angle of 7.3 (2°) with respect to the aniline ring, and at an angle of 55.6 (2°) with respect to the other phenyl ring. There is an intramolecular hydrogen bond involving the NH group and the carbonyl O atom. The crystal structure is stabilized by weak $\text{C}-\text{H}\cdots\pi$ interactions, which link the molecules into a herringbone arrangement.

Related literature

For related literature see: Dondoni & Perrone (1993); Ferraz *et al.* (1995); Michael *et al.* (2001); Azzaro *et al.* (1981); Alberola *et al.* (1999); Chaaban *et al.* (1979); Augusti & Kascheres (1993); Bejan *et al.* (1998); Eberlin & Kascheres (1988); Greenhill (1977); Michael *et al.* (1999); Elassar & El-Khair (2003); Zhang *et al.* (2006).



Experimental

Crystal data

 $\text{C}_{21}\text{H}_{17}\text{NO}$
 $M_r = 299.36$

 Monoclinic, $P2_1/c$
 $a = 15.880$ (7) Å
 $b = 6.034$ (3) Å
 $c = 18.401$ (8) Å
 $\beta = 114.433$ (7°)
 $V = 1605.4$ (13) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.08$ mm⁻¹
 $T = 294$ (2) K
 $0.24 \times 0.20 \times 0.14$ mm

Data collection

 Bruker SMART CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2000)
 $T_{\min} = 0.96$, $T_{\max} = 0.98$

 7511 measured reflections
 2774 independent reflections
 1580 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.051$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.079$
 $wR(F^2) = 0.249$
 $S = 1.04$
 2774 reflections

 209 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.24$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.23$ e Å⁻³
Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1}\cdots\text{O1}$	0.86	1.94	2.643 (5)	138
$\text{C18}-\text{H18}\cdots\text{Cg}^i$	0.93	2.84	3.627 (1)	142

 Symmetry code: (i) $-x + 1, y - \frac{1}{2}, -z + \frac{1}{2}$. Cg is the centroid of the C16-C21 ring.

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); 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: SU2060).

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supporting information

Acta Cryst. (2008). E64, o1327 [doi:10.1107/S1600536808016711]

(Z)-3-Anilino-1,3-diphenylprop-2-en-1-one

Li-Ping Zhang, Lin-Juan Wei, Ming-Qing Chen and Zhan-Hui Zhang

S1. Comment

β -enamino ketones are a highly versatile class of intermediates for the synthesis of natural therapeutic and biologically active analogues (Dondoni & Perrone, 1993; Ferraz *et al.*, 1995; Michael *et al.*, 2001; Azzaro *et al.*, 1981). Pyrroles, oxazoles, pyridinones, quinolines, dibenzodiazepines have also been prepared from enamines (Alberola *et al.*, 1999; Chaaban *et al.*, 1979; Augusti & Kascheres, 1993; Bejan *et al.*, 1998; Eberlin & Kascheres, 1988). It is therefore not surprising that many synthetic methods have been developed for the preparation of these compounds (Greenhill, 1977; Michael *et al.*, 1999; Elassar & El-Khair, 2003). During our development of new environmentally friendly methodologies for the preparation of β -enamino ketones (Zhang *et al.*, 2006), we synthesized the title compound, (I), the structure of which is reported here.

The molecular structure of compound (I) is illustrated in Fig. 1. The geometry of the enamine double bond is *Z*, with hydrogen bonding of the enamine N—H to the carbonyl oxygen atom (Table 1). Phenyl ring A (C1–C6) forms dihedral angles of 7.3 (2)° and 55.6 (2)° with the aniline ring C (C16–C21) and the phenyl ring B (C10–C15), respectively. As in other β -enamino ketones compound (I) displays electron delocalization, as shown by the comparison of the N1—C9 [1.347 (6)°] and N1—C16 [1.417 (6) Å] bond lengths.

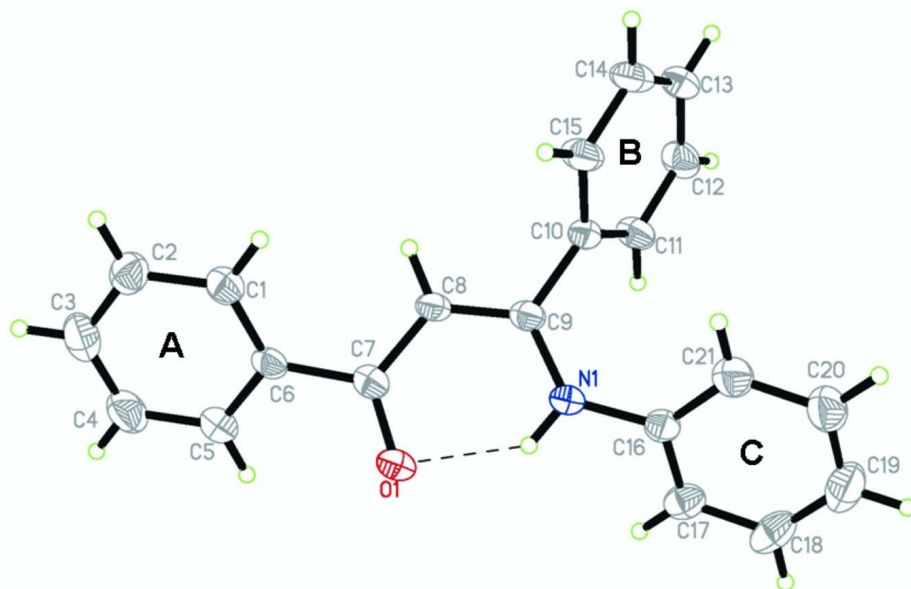
The crystal structure of compound (I) is stabilized by weak C—H \cdots π interactions, which link the molecules into a herringbone chain (Fig. 2). The distance of the H atom to the centroid of the benzene ring is 2.834 (10) Å.

S2. Experimental

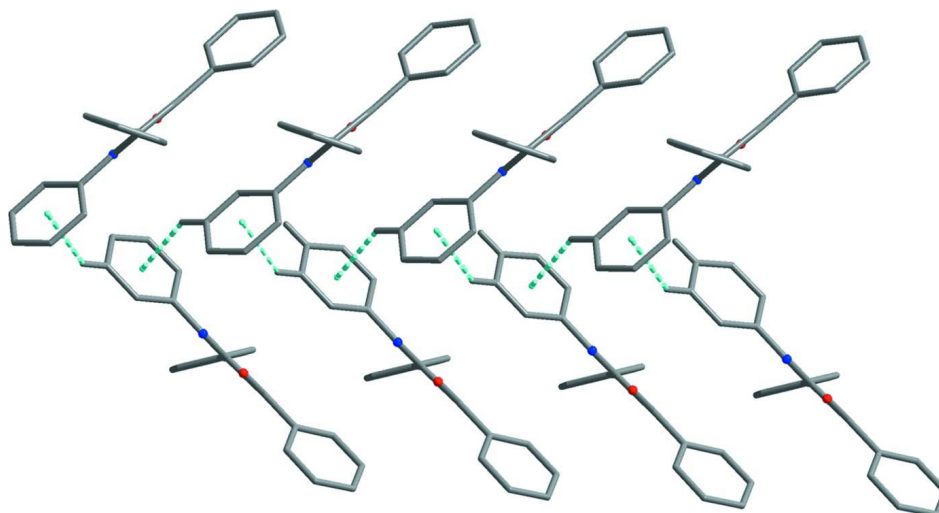
A mixture of the 1,3-diphenylpropane-1,3-dione (5 mmol), aniline (5 mmol) and InBr₃ (0.05 mmol) was stirred at room temperature for 6 h. After completion of the reaction, the reaction mixture was diluted with H₂O (10 ml) and extracted with EtOAc (210 ml). The combined organic layers were dried, concentrated, and then purified by column chromatography on SiO₂ with ethyl acetate-cyclohexane (1: 8), giving a yellow-orange solid (yield 68%). Mp 96–97°C; IR (neat, cm⁻¹): ν 3053, 1592, 1568, 1475, 1441, 1323, 1212, 1079, 1053, 1022, 904, 841, 697 ¹H NMR (CDCl₃, 300 MHz): δ 6.09 (s, 1H), 6.78 (d, 2H), 6.96–7.00 (m, 1H), 7.09–7.14 (m, 2H), 7.26–7.50 (m, 8H), 7.96 (d, 2H), 12.90 (br s, 1H, NH). ¹³C NMR (CDCl₃, 75 MHz): δ 97.0, 123.1, 124.2, 127.2, 128.2, 128.5, 128.7, 129.6, 131.3, 135.8, 139.4, 139.8, 161.4, 189.6. ESI-MS: 300 (*M*+1)⁺ Elemental Anal. Calcd. for C₂₁H₁₇NO: C, 84.25; H, 5.72; N, 4.68. Found: C, 84.48; H, 5.82; N, 4.45. Single crystals of (I), suitable for X-ray diffraction analysis, were obtained from ethyl acetate-cyclohexane by slow evaporation at room temperature.

S3. Refinement

H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with N—H = 0.86 Å, C—H = 0.93 - 0.97 Å, and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{CH}_3)$ or $1.2U_{\text{eq}}(\text{C}, \text{N})$.

**Figure 1**

The molecular structure of compound (I), showing the atomic numbering scheme and the displacement ellipsoids drawn at the 30% probability level. The intramolecular N-H \cdots O hydrogen bond is shown as a dashed line.

**Figure 2**

The molecular packing of compound (I), showing the C—H \cdots π interactions (dashed lines).

(Z)-3-Anilino-1,3-diphenylprop-2-en-1-one

Crystal data

$C_{21}H_{17}NO$

$M_r = 299.36$

Monoclinic, $P2_1/c$

Hall symbol: $-P 2_1/c$

$a = 15.880 (7) \text{ \AA}$

$b = 6.034 (3) \text{ \AA}$

$c = 18.401 (8) \text{ \AA}$

$\beta = 114.433 (7)^\circ$

$V = 1605.4 (13) \text{ \AA}^3$
 $Z = 4$
 $F(000) = 632$
 $D_x = 1.239 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
 Cell parameters from 1702 reflections

$\theta = 2.3\text{--}23.8^\circ$
 $\mu = 0.08 \text{ mm}^{-1}$
 $T = 294 \text{ K}$
 Block, yellow
 $0.24 \times 0.20 \times 0.14 \text{ mm}$

Data collection

Bruker SMART CCD area-detector
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 phi and ω scans
 Absorption correction: multi-scan
 (SADABS; Bruker, 2000)
 $T_{\min} = 0.96, T_{\max} = 0.98$

7511 measured reflections
 2774 independent reflections
 1580 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.052$
 $\theta_{\text{max}} = 25.0^\circ, \theta_{\text{min}} = 2.3^\circ$
 $h = -17 \rightarrow 18$
 $k = -7 \rightarrow 7$
 $l = -17 \rightarrow 21$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.079$
 $wR(F^2) = 0.249$
 $S = 1.05$
 2774 reflections
 209 parameters
 0 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
 $w = 1/[\sigma^2(F_o^2) + (0.1119P)^2 + 1.614P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.24 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.23 \text{ e \AA}^{-3}$
 Extinction correction: SHELXL97,
 $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.021 (4)

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 $F^2 > \sigma(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.2315 (2)	0.0638 (5)	0.19524 (16)	0.0578 (9)
N1	0.3124 (2)	-0.1522 (6)	0.11657 (19)	0.0490 (9)
H1	0.3021	-0.1332	0.1585	0.059*
C1	0.1066 (3)	0.5369 (7)	0.0895 (2)	0.0511 (11)
H1A	0.1389	0.5646	0.0582	0.061*
C2	0.0442 (3)	0.6921 (8)	0.0932 (3)	0.0616 (13)
H2	0.0358	0.8249	0.0654	0.074*
C3	-0.0053 (3)	0.6511 (10)	0.1376 (3)	0.0723 (16)
H3	-0.0474	0.7553	0.1396	0.087*

C4	0.0075 (4)	0.4553 (11)	0.1792 (3)	0.0750 (16)
H4	-0.0267	0.4262	0.2087	0.090*
C5	0.0711 (3)	0.3018 (9)	0.1771 (3)	0.0586 (13)
H5	0.0804	0.1709	0.2061	0.070*
C6	0.1212 (3)	0.3424 (7)	0.1318 (2)	0.0430 (10)
C7	0.1904 (3)	0.1718 (7)	0.1323 (2)	0.0451 (10)
C8	0.2038 (3)	0.1350 (7)	0.0618 (2)	0.0435 (10)
H8	0.1709	0.2233	0.0177	0.052*
C9	0.2619 (3)	-0.0218 (7)	0.0543 (2)	0.0421 (10)
C10	0.2628 (3)	-0.0622 (7)	-0.0250 (2)	0.0418 (10)
C11	0.2382 (3)	-0.2677 (8)	-0.0616 (2)	0.0521 (12)
H11	0.2253	-0.3840	-0.0346	0.063*
C12	0.2325 (3)	-0.3011 (8)	-0.1375 (2)	0.0585 (13)
H12	0.2151	-0.4388	-0.1619	0.070*
C13	0.2526 (3)	-0.1323 (9)	-0.1769 (3)	0.0611 (13)
H13	0.2491	-0.1554	-0.2281	0.073*
C14	0.2776 (4)	0.0702 (9)	-0.1418 (3)	0.0690 (15)
H14	0.2913	0.1846	-0.1690	0.083*
C15	0.2828 (3)	0.1064 (8)	-0.0654 (3)	0.0587 (13)
H15	0.2997	0.2450	-0.0418	0.070*
C16	0.3797 (3)	-0.3154 (7)	0.1242 (2)	0.0458 (11)
C17	0.3834 (3)	-0.5000 (7)	0.1687 (2)	0.0536 (12)
H17	0.3408	-0.5166	0.1910	0.064*
C18	0.4486 (4)	-0.6602 (8)	0.1808 (3)	0.0679 (15)
H18	0.4510	-0.7834	0.2120	0.082*
C19	0.5104 (4)	-0.6391 (10)	0.1473 (3)	0.0804 (17)
H19	0.5539	-0.7497	0.1544	0.096*
C20	0.5083 (3)	-0.4551 (12)	0.1031 (3)	0.0783 (17)
H20	0.5509	-0.4409	0.0807	0.094*
C21	0.4432 (3)	-0.2894 (9)	0.0914 (3)	0.0647 (13)
H21	0.4424	-0.1633	0.0620	0.078*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.077 (2)	0.063 (2)	0.0374 (15)	0.0107 (17)	0.0279 (15)	0.0051 (15)
N1	0.062 (2)	0.054 (2)	0.0368 (17)	0.0121 (18)	0.0251 (17)	0.0093 (16)
C1	0.056 (3)	0.053 (3)	0.047 (2)	-0.005 (2)	0.023 (2)	-0.006 (2)
C2	0.067 (3)	0.053 (3)	0.056 (3)	0.005 (2)	0.016 (2)	-0.007 (2)
C3	0.058 (3)	0.091 (4)	0.064 (3)	0.012 (3)	0.021 (3)	-0.023 (3)
C4	0.069 (3)	0.104 (5)	0.065 (3)	0.013 (3)	0.041 (3)	-0.002 (3)
C5	0.068 (3)	0.066 (3)	0.048 (2)	0.004 (3)	0.031 (2)	0.000 (2)
C6	0.051 (2)	0.046 (2)	0.0301 (19)	-0.0043 (19)	0.0157 (18)	-0.0060 (17)
C7	0.051 (2)	0.047 (3)	0.040 (2)	-0.005 (2)	0.0211 (19)	-0.0032 (19)
C8	0.054 (2)	0.047 (2)	0.0299 (19)	0.002 (2)	0.0177 (18)	0.0031 (18)
C9	0.050 (2)	0.044 (2)	0.0333 (19)	-0.001 (2)	0.0178 (18)	0.0006 (18)
C10	0.047 (2)	0.045 (2)	0.0315 (19)	0.0042 (19)	0.0152 (18)	0.0012 (17)
C11	0.070 (3)	0.050 (3)	0.041 (2)	-0.006 (2)	0.028 (2)	-0.004 (2)

C12	0.071 (3)	0.061 (3)	0.044 (2)	-0.004 (2)	0.024 (2)	-0.015 (2)
C13	0.078 (3)	0.073 (4)	0.038 (2)	0.012 (3)	0.029 (2)	0.003 (2)
C14	0.104 (4)	0.067 (4)	0.051 (3)	0.009 (3)	0.046 (3)	0.017 (3)
C15	0.094 (4)	0.046 (3)	0.047 (2)	0.000 (2)	0.040 (3)	0.004 (2)
C16	0.048 (2)	0.051 (3)	0.033 (2)	0.002 (2)	0.0113 (18)	-0.0049 (18)
C17	0.055 (3)	0.049 (3)	0.045 (2)	-0.004 (2)	0.008 (2)	-0.003 (2)
C18	0.068 (3)	0.042 (3)	0.068 (3)	0.004 (3)	0.002 (3)	0.002 (2)
C19	0.068 (4)	0.076 (4)	0.078 (4)	0.024 (3)	0.011 (3)	-0.012 (3)
C20	0.057 (3)	0.114 (5)	0.064 (3)	0.016 (3)	0.025 (3)	-0.003 (3)
C21	0.056 (3)	0.084 (4)	0.056 (3)	0.007 (3)	0.024 (2)	0.006 (3)

Geometric parameters (Å, °)

O1—C7	1.252 (5)	C10—C11	1.388 (6)
N1—C9	1.347 (5)	C11—C12	1.377 (6)
N1—C16	1.416 (5)	C11—H11	0.9300
N1—H1	0.8600	C12—C13	1.362 (6)
C1—C6	1.373 (6)	C12—H12	0.9300
C1—C2	1.386 (6)	C13—C14	1.362 (7)
C1—H1A	0.9300	C13—H13	0.9300
C2—C3	1.369 (7)	C14—C15	1.391 (6)
C2—H2	0.9300	C14—H14	0.9300
C3—C4	1.377 (8)	C15—H15	0.9300
C3—H3	0.9300	C16—C17	1.369 (6)
C4—C5	1.382 (7)	C16—C21	1.384 (6)
C4—H4	0.9300	C17—C18	1.366 (7)
C5—C6	1.393 (6)	C17—H17	0.9300
C5—H5	0.9300	C18—C19	1.363 (8)
C6—C7	1.502 (6)	C18—H18	0.9300
C7—C8	1.416 (5)	C19—C20	1.369 (8)
C8—C9	1.368 (6)	C19—H19	0.9300
C8—H8	0.9300	C20—C21	1.389 (7)
C9—C10	1.486 (5)	C20—H20	0.9300
C10—C15	1.372 (6)	C21—H21	0.9300
C9—N1—C16	130.5 (3)	C12—C11—C10	120.6 (4)
C9—N1—H1	114.7	C12—C11—H11	119.7
C16—N1—H1	114.7	C10—C11—H11	119.7
C6—C1—C2	120.4 (4)	C13—C12—C11	119.9 (4)
C6—C1—H1A	119.8	C13—C12—H12	120.0
C2—C1—H1A	119.8	C11—C12—H12	120.0
C3—C2—C1	120.4 (5)	C12—C13—C14	120.3 (4)
C3—C2—H2	119.8	C12—C13—H13	119.8
C1—C2—H2	119.8	C14—C13—H13	119.8
C2—C3—C4	119.8 (5)	C13—C14—C15	120.2 (4)
C2—C3—H3	120.1	C13—C14—H14	119.9
C4—C3—H3	120.1	C15—C14—H14	119.9
C3—C4—C5	120.1 (5)	C10—C15—C14	120.1 (4)

C3—C4—H4	120.0	C10—C15—H15	120.0
C5—C4—H4	120.0	C14—C15—H15	120.0
C4—C5—C6	120.3 (5)	C17—C16—C21	119.7 (4)
C4—C5—H5	119.9	C17—C16—N1	118.0 (4)
C6—C5—H5	119.9	C21—C16—N1	122.3 (4)
C1—C6—C5	119.0 (4)	C18—C17—C16	121.1 (5)
C1—C6—C7	122.8 (4)	C18—C17—H17	119.5
C5—C6—C7	118.3 (4)	C16—C17—H17	119.5
O1—C7—C8	123.2 (4)	C19—C18—C17	119.9 (5)
O1—C7—C6	117.5 (3)	C19—C18—H18	120.0
C8—C7—C6	119.3 (4)	C17—C18—H18	120.0
C9—C8—C7	124.4 (4)	C18—C19—C20	120.0 (5)
C9—C8—H8	117.8	C18—C19—H19	120.0
C7—C8—H8	117.8	C20—C19—H19	120.0
N1—C9—C8	120.4 (3)	C19—C20—C21	120.6 (5)
N1—C9—C10	119.7 (4)	C19—C20—H20	119.7
C8—C9—C10	119.6 (3)	C21—C20—H20	119.7
C15—C10—C11	118.8 (4)	C16—C21—C20	118.7 (5)
C15—C10—C9	120.6 (4)	C16—C21—H21	120.6
C11—C10—C9	120.5 (4)	C20—C21—H21	120.6
C6—C1—C2—C3	-1.5 (7)	N1—C9—C10—C11	56.6 (6)
C1—C2—C3—C4	0.4 (7)	C8—C9—C10—C11	-117.8 (5)
C2—C3—C4—C5	0.9 (8)	C15—C10—C11—C12	-0.9 (7)
C3—C4—C5—C6	-1.2 (7)	C9—C10—C11—C12	175.3 (4)
C2—C1—C6—C5	1.2 (6)	C10—C11—C12—C13	1.0 (7)
C2—C1—C6—C7	-177.8 (4)	C11—C12—C13—C14	-0.4 (8)
C4—C5—C6—C1	0.2 (6)	C12—C13—C14—C15	-0.1 (8)
C4—C5—C6—C7	179.2 (4)	C11—C10—C15—C14	0.3 (7)
C1—C6—C7—O1	146.2 (4)	C9—C10—C15—C14	-175.9 (4)
C5—C6—C7—O1	-32.8 (6)	C13—C14—C15—C10	0.2 (8)
C1—C6—C7—C8	-35.9 (6)	C9—N1—C16—C17	-143.8 (4)
C5—C6—C7—C8	145.0 (4)	C9—N1—C16—C21	38.9 (7)
O1—C7—C8—C9	0.5 (7)	C21—C16—C17—C18	-0.4 (6)
C6—C7—C8—C9	-177.2 (4)	N1—C16—C17—C18	-177.7 (4)
C16—N1—C9—C8	-176.4 (4)	C16—C17—C18—C19	-1.1 (7)
C16—N1—C9—C10	9.3 (7)	C17—C18—C19—C20	1.6 (8)
C7—C8—C9—N1	-1.0 (6)	C18—C19—C20—C21	-0.5 (8)
C7—C8—C9—C10	173.4 (4)	C17—C16—C21—C20	1.4 (7)
N1—C9—C10—C15	-127.2 (5)	N1—C16—C21—C20	178.6 (4)
C8—C9—C10—C15	58.4 (6)	C19—C20—C21—C16	-0.9 (8)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N1—H1 \cdots O1	0.86	1.94	2.643 (5)	138

C18—H18 \cdots Cg ⁱ	0.93	2.84	3.627 (1)	142
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Symmetry code: (i) $-x+1, y-1/2, -z+1/2$.