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Crystal structure of 1-{4-hydroxy-3-[(pyrrolidin-1-yl)methyl]phenyl}-3-phenylprop-2-en-1-one

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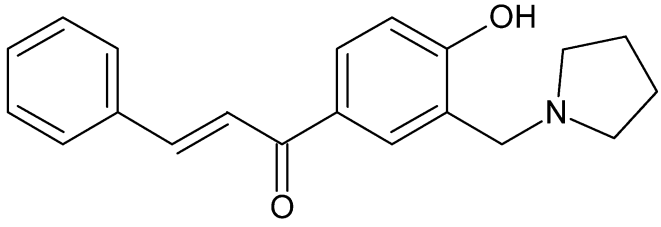
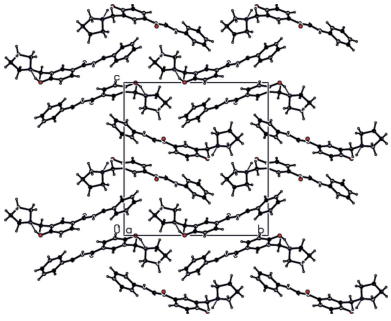
In the title compound, $C_{20}H_{21}NO_2$, the pyrrolidine ring adopts an envelope conformation with the N atom at the flap position. The central benzene ring makes dihedral angles of 21.39 (10) and 80.10 (15)° with the phenyl ring and the mean plane of the pyrrolidine ring, respectively. The molecular conformation is stabilized by an intramolecular O—H···N hydrogen bond, which closes an $S(6)$ ring. A weak C—H···π interaction is observed in the crystal.

1. Chemical context

Mannich bases are a group of compounds having various biological activities such as cytotoxic (Bilginer *et al.*, 2013), anti-inflammatory (Sahin *et al.*, 2010) and anticonvulsant (Gul *et al.*, 2004) activities. α,β-Unsaturated ketones present in the chemical structure of Mannich bases themselves or those produced from them by deamination processes are responsible for their cytotoxicity.



The cytotoxic and anticancer properties of chalcone (1,3-diphenyl-2-propenone) and related compounds have been reported (Bilginer *et al.*, 2013; Dimmock *et al.*, 1998; Gul Cizmecioglu *et al.*, 2009); Gul Mete *et al.*, 2009). The title compound, (I), reported in this study is a Mannich base of phenolic chalcone.



2. Structural commentary

In the title compound (Fig. 1), the pyrrolidine ring (N1/C17–C20) exhibits an envelope conformation with the N atom at the flap position [the puckering parameters are $Q(2)$ = 0.350 (3) Å and $\varphi(2)$ = 186.9 (5)°]. The central benzene ring (C10–C15) makes dihedral angles of 21.39 (10) and 80.10 (15)°, with the phenyl ring (C1–C6) and the mean plane of the pyrrolidine ring (N1/C17–C20), respectively. Otherwise, the geometrical parameters for (I) are comparable those

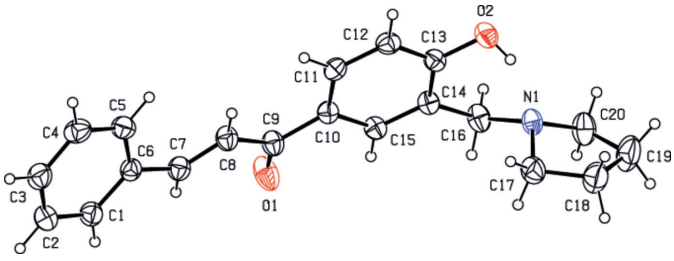


Figure 1
View of the molecular structure of the title compound, with displacement ellipsoids drawn at the 30% probability level.

reported for related compounds (Suhud *et al.*, 2015; Palakshamurthy *et al.*, 2012). An intramolecular O2—H1*O*···N1 hydrogen bond (Table 1, Fig. 2) helps to establish the molecular conformation of (I).

3. Supramolecular features

The only directional interaction present in the crystal of (I) is a very weak C—H···π bond (Table 1).

4. Semi-empirical quantum-mechanical calculations

A theoretical calculation was carried out using the semi-empirical quantum-mechanical *CNDO/2* (Complete Neglect of Differential Overlap) method (Pople & Beveridge, 1970). The spatial view of the single molecule, with atomic labels, calculated as a closed-shell in a vacuum is shown in Fig. 3. The charges at atoms O1, O2 and N1 are −0.337, −0.271 and −0.159 e^{-}, respectively. The calculated dipole moment is 2.760 Debye.

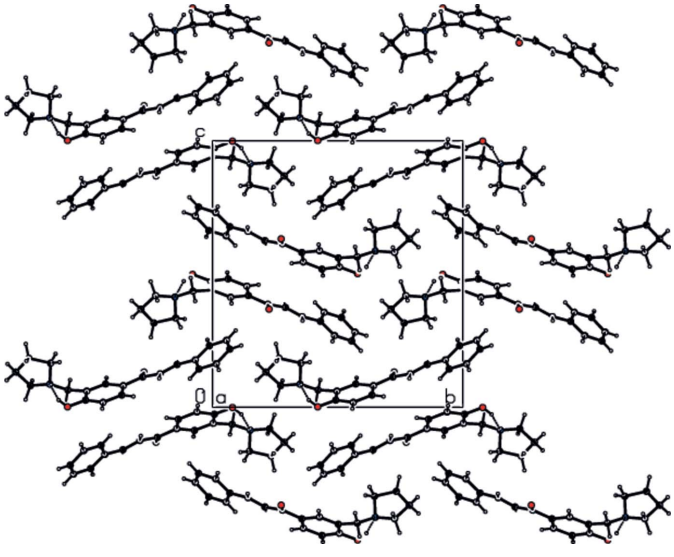


Figure 2
The molecular packing and hydrogen bonding viewed down the *a* axis.

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

*Cg*3 is the centroid of the C10–C15 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H1*O*···N1	0.85 (3)	1.85 (3)	2.633 (2)	154 (3)
C5—H5···*Cg*3^{i}	0.93	2.99	3.685 (2)	132

Symmetry code: (i) $x+\frac{1}{2}, -y+\frac{3}{2}, -z$.

5. Biological activity

Compound (I) was tested against human hepatoma (Huh7) and breast cancer cell (T47D) lines in terms of its cytotoxic activities, and showed activities against both cell lines used, especially against the T47D cell line. The compound studied here may serve as a model compound for designing new anticancer compounds for further studies (Yerdelen, 2009).

6. Synthesis and crystallization

A solution of paraformaldehyde (0.132 g; 4.4 mmol) and pyrrolidine (0.317 g, 4.4 mmol) in acetonitrile (5 mL) was heated under reflux at 353 K for 30 min. A solution of the chalcone, 1-(4-hydroxyphenyl)-3-phenyl-2-propen-1-one (1 g, 4.4 mmol) in acetonitrile (25 ml), was added to the reaction flask and heating was continued. The reaction was monitored by thin layer chromatography (TLC) and stopped after 7.5 h. The reaction solvent was distilled under vacuum. The residue was purified by column chromatography using Al_2O_3 as adsorbant and $CHCl_3$/MeOH (9:1) as eluent. The title compound was obtained in 44% yield (m.p. = 398–402 K).Crystals suitable for X-ray diffaction analysis were obtained by recrystallization from ehanol.

^{1}H NMR ($CDCl_3$, p.p.m.) δ 1.89–1.86 (*m*, 4H, C18-H, C19-H); 2.67 (*br s*, 4H, C17-H, C20-H); 3.90 (*s*, 2H, C16-H); 6.88–6.86 (*d*, 1H, C14-H); 7.41–7.39 (*m*, 3H, C3-H, C4-H, C5-H); 7.56–7.53 (*d*, 1H, C8-H, *J* = 15.4 Hz); 7.65–7.62 (*m*, 2H, C2-H, C6-H); 7.78–7.77 (*d*, 1H, C11-H); 7.80–7.76 (*d*, 1H, C7-H, *J* = 15.4 Hz); 7.92–7.90 (*dd*, 1H, C15-H);

^{13}C NMR ($CDCl_3$, p.p.m.) δ 188.82 (C9), 163.59 (C13), 143.77 (C7), 135.42 (C1), 130.43 (C11), 130.39 (C15), 129.60 (C10), 129.25 (C3, C5), 129.12 (C4), 128.55 (C2, C6), 122.68 (C12), 122.16 (C8), 116.15 (C14), 50.80 (C16), 53.69 (C17,

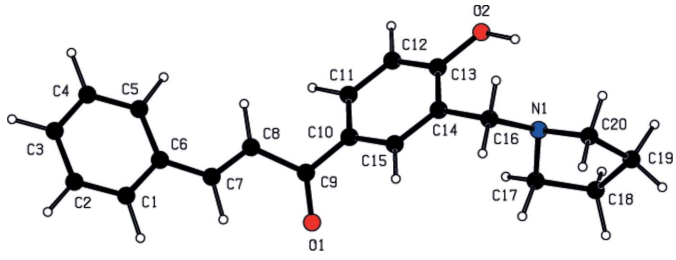


Figure 3
The conformation of the title compound, calculated using the *CNDO* method.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{20}H_{21}NO_2$
M_r	307.38
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	296
a, b, c (Å)	5.8403 (5), 16.3195 (13), 17.3615 (14)
V (Å^3)	1654.7 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.66 × 0.53 × 0.33
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2007)
T_{min}, T_{max}	0.951, 0.974
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	37526, 4120, 3647
R_{int}	0.050
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.668
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.043, 0.118, 1.03
No. of reflections	4120
No. of parameters	211
No. of restraints	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.24, −0.12

Computer programs: *APEX2* and *SAINT* (Bruker, 2007), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009).

C20), 23.88 (C18, C19); TOF MS [ES (−)] ($CHCl_3$) m/z: M^+ (307.15), M^+-1 (306.15) (Yerdelen, 2009).

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Carbon-bound H atoms were placed in calculated positions with C—H = 0.93 and 0.97 Å, and refined using a riding model with U_{iso}(H) = 1.2U_{eq}(C). The hydroxyl H atom was found from a difference Fourier map and its positional parameters were freely refined with U_{iso}(H) = 1.5U_{eq}(O). The most disagreeable reflections (2 4 0), (4 9 0), (4 12 0), (5 12 4), (3 12 5), (3 3 1), (0 16 5), (1 3 0), (2 20 6), (−2 13 17), (0 5 4), (0 11 4) and (2 13 4) were omitted in the final cycles of refinement. The Flack absolute structure parameter was found to be indeterminate in the present study.

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References

Bilginer, S., Gul, H. I., Mete, E., Das, U., Sakagami, H., Umemura, N. & Dimmock, J. R. (2013). *J. Enzyme Inhib. Med. Chem.* **28**, 974–980.
Bruker (2007). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Dimmock, J. R., Kandepu, N. M., Hetherington, M., Quail, J. W., Pugazhenthi, U., Sudom, A. M., Chamankhah, M., Rose, P., Pass, E., Allen, T. M., Halleran, S., Szydlowski, J., Mutus, B., Tannous, M., Manavathu, E. K., Myers, T. G., De Clercq, E. & Balzarini, J. (1998). *J. Med. Chem.* **41**, 1014–1026.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Gul, H. I., Calis, U. & Vepsalainen, J. (2004). *Arzn. Fors.* **54**, 359–364.
Gul, H. I., Cizmecioglu, M., Zencir, S., Gul, M., Canturk, P., Atalay, M. & Topcu, Z. (2009). *J. Enzyme Inhib. Med. Chem.* **24**, 804–807.
Gul, M., Mete, E., Atalay, M., Arik, M. & Gul, H. I. (2009). *Arzn. Fors. Drug. Res.* , **59**, 364–369.
Palakshamurthy, B. S., Srinivasa, H. T., Kumar, V., Sreenivasa, S. & Devarajegowda, H. C. (2012). *Acta Cryst.* E**68**, o3382.
Pople, J. A. & Beveridge, D. L. (1970). In *Approximate Molecular Orbital Theory*. New York: McGraw–Hill.
Sahin, Y. N., Demircan, B., Suleyman, H., Aksoy, H. & Gul, H. I. (2010). *Turk. J. Med. Sci.* **40**, 723–728.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Suhud, K., Heng, L. Y., Hasbullah, S. A., Ahmad, M. & Kassim, M. B. (2015). *Acta Cryst.* E**71**, o225–o226.
Yerdelen, K. O. (2009). PhD thesis, Health Sciences, Atatürk University, Erzurum, Turkey.

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Computing details

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2009).

1-{4-Hydroxy-3-[(pyrrolidin-1-yl)methyl]phenyl}-3-phenylprop-2-en-1-one

Crystal data

$C_{20}H_{21}NO_2$
$M_r = 307.38$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 5.8403$ (5) Å
$b = 16.3195$ (13) Å
$c = 17.3615$ (14) Å
$V = 1654.7$ (2) Å^3
$Z = 4$
$F(000) = 656$
$D_x = 1.234$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4120 reflections
$\theta = 2.4$–$27.7°$
$\mu = 0.08$ mm^{-1}
$T = 296$ K
Prism, light yellow
0.66 × 0.53 × 0.33 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
$T_{min} = 0.951$, $T_{max} = 0.974$
37526 measured reflections
4120 independent reflections
3647 reflections with $I > 2\sigma(I)$
$R_{int} = 0.050$
$\theta_{max} = 28.4°$, $\theta_{min} = 1.7°$
$h = -7 \rightarrow 7$
$k = -21 \rightarrow 21$
$l = -23 \rightarrow 23$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.118$
$S = 1.03$
4120 reflections
211 parameters
1 restraint
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.068P)^2 + 0.1361P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.12$ e Å^{-3}

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating -R-factor-obs 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	−0.0436 (3)	0.72582 (11)	0.13185 (14)	0.0800 (7)
O2	0.4920 (3)	0.42033 (9)	0.00124 (10)	0.0578 (5)
N1	0.1759 (3)	0.34948 (10)	0.08639 (10)	0.0495 (5)
C1	0.3003 (4)	0.98751 (12)	0.23067 (13)	0.0524 (6)
C2	0.4274 (5)	1.05592 (14)	0.25148 (13)	0.0607 (7)
C3	0.6363 (4)	1.06897 (14)	0.21774 (14)	0.0610 (7)
C4	0.7188 (4)	1.01504 (15)	0.16329 (13)	0.0602 (7)
C5	0.5935 (4)	0.94596 (13)	0.14348 (12)	0.0534 (6)
C6	0.3823 (3)	0.93109 (11)	0.17767 (10)	0.0443 (5)
C7	0.2469 (4)	0.85825 (12)	0.15995 (12)	0.0498 (6)
C8	0.3149 (4)	0.79067 (12)	0.12533 (12)	0.0511 (6)
C9	0.1583 (4)	0.72064 (12)	0.11351 (13)	0.0499 (6)
C10	0.2497 (3)	0.64318 (11)	0.08086 (10)	0.0431 (5)
C11	0.4636 (4)	0.63705 (12)	0.04543 (11)	0.0466 (6)
C12	0.5411 (4)	0.56234 (13)	0.01826 (11)	0.0495 (6)
C13	0.4084 (3)	0.49271 (12)	0.02654 (11)	0.0441 (5)
C14	0.1907 (3)	0.49728 (11)	0.06048 (11)	0.0433 (5)
C15	0.1167 (3)	0.57238 (12)	0.08719 (11)	0.0441 (5)
C16	0.0423 (4)	0.42179 (13)	0.06449 (14)	0.0550 (6)
C17	0.2614 (5)	0.35266 (14)	0.16535 (14)	0.0648 (8)
C18	0.3247 (6)	0.26561 (15)	0.18383 (17)	0.0787 (10)
C19	0.1771 (7)	0.21350 (17)	0.1318 (2)	0.0941 (13)
C20	0.0483 (5)	0.27222 (14)	0.08114 (18)	0.0719 (9)
H1	0.15700	0.97930	0.25270	0.0630*
H1O	0.418 (6)	0.3850 (16)	0.0268 (18)	0.0870*
H2	0.37130	1.09250	0.28800	0.0730*
H3	0.72280	1.11450	0.23160	0.0730*
H4	0.85910	1.02500	0.13970	0.0720*
H5	0.65110	0.90950	0.10720	0.0640*
H7	0.09410	0.85980	0.17490	0.0600*
H8	0.46510	0.78690	0.10790	0.0610*
H11	0.55450	0.68350	0.04010	0.0560*
H12	0.68320	0.55890	−0.00570	0.0590*
H15	−0.02670	0.57600	0.11020	0.0530*
H16A	−0.07880	0.43040	0.10190	0.0660*

H16B	−0.02830	0.41250	0.01470	0.0660*
H17A	0.14400	0.37250	0.20020	0.0780*
H17B	0.39400	0.38830	0.16900	0.0780*
H18A	0.29390	0.25340	0.23750	0.0950*
H18B	0.48580	0.25600	0.17360	0.0950*
H19A	0.27120	0.17710	0.10100	0.1130*
H19B	0.07160	0.18070	0.16200	0.1130*
H20A	0.04430	0.25260	0.02840	0.0860*
H20B	−0.10750	0.27930	0.09930	0.0860*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0507 (9)	0.0596 (10)	0.1298 (18)	−0.0041 (7)	0.0166 (10)	−0.0278 (10)
O2	0.0555 (9)	0.0515 (8)	0.0663 (9)	0.0081 (7)	0.0056 (7)	−0.0088 (7)
N1	0.0488 (9)	0.0383 (8)	0.0613 (10)	−0.0074 (7)	−0.0064 (8)	−0.0087 (7)
C1	0.0520 (11)	0.0477 (10)	0.0574 (11)	−0.0010 (9)	0.0031 (10)	0.0005 (9)
C2	0.0739 (15)	0.0497 (11)	0.0586 (12)	−0.0030 (11)	0.0022 (11)	−0.0077 (9)
C3	0.0712 (15)	0.0524 (11)	0.0593 (12)	−0.0158 (11)	−0.0055 (11)	−0.0015 (10)
C4	0.0575 (13)	0.0671 (13)	0.0559 (11)	−0.0157 (11)	0.0028 (10)	0.0035 (10)
C5	0.0567 (12)	0.0548 (11)	0.0488 (10)	−0.0026 (9)	0.0032 (9)	−0.0034 (8)
C6	0.0480 (10)	0.0419 (9)	0.0431 (9)	0.0014 (8)	−0.0052 (7)	0.0033 (7)
C7	0.0475 (10)	0.0472 (10)	0.0547 (10)	−0.0015 (8)	−0.0001 (8)	0.0017 (8)
C8	0.0485 (11)	0.0450 (10)	0.0598 (11)	−0.0021 (8)	0.0000 (9)	−0.0025 (8)
C9	0.0444 (10)	0.0447 (10)	0.0607 (11)	−0.0001 (8)	−0.0013 (9)	−0.0034 (8)
C10	0.0427 (9)	0.0421 (9)	0.0446 (9)	0.0006 (8)	−0.0046 (7)	0.0001 (7)
C11	0.0442 (9)	0.0466 (10)	0.0490 (10)	−0.0057 (8)	0.0012 (8)	0.0048 (8)
C12	0.0407 (9)	0.0584 (11)	0.0493 (10)	0.0036 (9)	0.0068 (8)	0.0028 (8)
C13	0.0434 (10)	0.0459 (9)	0.0431 (8)	0.0052 (8)	−0.0032 (8)	−0.0026 (7)
C14	0.0388 (9)	0.0432 (9)	0.0478 (9)	−0.0009 (7)	−0.0065 (8)	−0.0035 (7)
C15	0.0339 (8)	0.0475 (9)	0.0510 (9)	0.0004 (7)	0.0005 (7)	−0.0029 (8)
C16	0.0424 (10)	0.0486 (10)	0.0741 (13)	−0.0049 (9)	−0.0064 (9)	−0.0110 (10)
C17	0.0794 (16)	0.0539 (12)	0.0610 (12)	−0.0079 (12)	−0.0102 (12)	−0.0087 (10)
C18	0.100 (2)	0.0572 (13)	0.0788 (16)	−0.0084 (14)	−0.0123 (17)	0.0062 (12)
C19	0.129 (3)	0.0513 (13)	0.102 (2)	−0.0247 (16)	−0.024 (2)	0.0075 (14)
C20	0.0704 (15)	0.0492 (12)	0.0960 (19)	−0.0208 (11)	−0.0125 (14)	−0.0097 (12)

Geometric parameters (Å, º)

O1—C9	1.224 (3)	C17—C18	1.503 (3)
O2—C13	1.352 (2)	C18—C19	1.511 (5)
N1—C16	1.465 (3)	C19—C20	1.503 (4)
N1—C17	1.460 (3)	C1—H1	0.9300
N1—C20	1.467 (3)	C2—H2	0.9300
O2—H1O	0.85 (3)	C3—H3	0.9300
C1—C2	1.389 (3)	C4—H4	0.9300
C1—C6	1.387 (3)	C5—H5	0.9300
C2—C3	1.370 (4)	C7—H7	0.9300

C3—C4	1.379 (3)	C8—H8	0.9300
C4—C5	1.387 (3)	C11—H11	0.9300
C5—C6	1.390 (3)	C12—H12	0.9300
C6—C7	1.461 (3)	C15—H15	0.9300
C7—C8	1.317 (3)	C16—H16A	0.9700
C8—C9	1.478 (3)	C16—H16B	0.9700
C9—C10	1.485 (3)	C17—H17A	0.9700
C10—C15	1.397 (3)	C17—H17B	0.9700
C10—C11	1.396 (3)	C18—H18A	0.9700
C11—C12	1.383 (3)	C18—H18B	0.9700
C12—C13	1.383 (3)	C19—H19A	0.9700
C13—C14	1.403 (3)	C19—H19B	0.9700
C14—C15	1.380 (3)	C20—H20A	0.9700
C14—C16	1.508 (3)	C20—H20B	0.9700

C16—N1—C17	113.41 (17)	C3—C4—H4	120.00
C16—N1—C20	113.92 (18)	C5—C4—H4	120.00
C17—N1—C20	105.22 (19)	C4—C5—H5	120.00
C13—O2—H1O	104 (2)	C6—C5—H5	120.00
C2—C1—C6	121.5 (2)	C6—C7—H7	116.00
C1—C2—C3	119.3 (2)	C8—C7—H7	116.00
C2—C3—C4	120.4 (2)	C7—C8—H8	119.00
C3—C4—C5	120.3 (2)	C9—C8—H8	119.00
C4—C5—C6	120.27 (19)	C10—C11—H11	120.00
C1—C6—C7	119.54 (18)	C12—C11—H11	120.00
C5—C6—C7	122.18 (17)	C11—C12—H12	120.00
C1—C6—C5	118.28 (18)	C13—C12—H12	120.00
C6—C7—C8	127.9 (2)	C10—C15—H15	119.00
C7—C8—C9	121.6 (2)	C14—C15—H15	119.00
O1—C9—C8	120.43 (19)	N1—C16—H16A	109.00
O1—C9—C10	120.29 (19)	N1—C16—H16B	109.00
C8—C9—C10	119.27 (19)	C14—C16—H16A	109.00
C9—C10—C11	123.43 (17)	C14—C16—H16B	109.00
C9—C10—C15	118.32 (17)	H16A—C16—H16B	108.00
C11—C10—C15	118.24 (17)	N1—C17—H17A	111.00
C10—C11—C12	120.41 (19)	N1—C17—H17B	111.00
C11—C12—C13	120.4 (2)	C18—C17—H17A	111.00
O2—C13—C12	118.81 (17)	C18—C17—H17B	111.00
O2—C13—C14	120.68 (17)	H17A—C17—H17B	109.00
C12—C13—C14	120.51 (18)	C17—C18—H18A	111.00
C13—C14—C15	118.17 (17)	C17—C18—H18B	111.00
C13—C14—C16	119.78 (17)	C19—C18—H18A	111.00
C15—C14—C16	122.02 (17)	C19—C18—H18B	111.00
C10—C15—C14	122.29 (17)	H18A—C18—H18B	109.00
N1—C16—C14	111.35 (18)	C18—C19—H19A	111.00
N1—C17—C18	104.54 (19)	C18—C19—H19B	110.00
C17—C18—C19	105.3 (2)	C20—C19—H19A	111.00
C18—C19—C20	106.1 (2)	C20—C19—H19B	111.00

N1—C20—C19	104.9 (2)	H19A—C19—H19B	109.00
C2—C1—H1	119.00	N1—C20—H20A	111.00
C6—C1—H1	119.00	N1—C20—H20B	111.00
C1—C2—H2	120.00	C19—C20—H20A	111.00
C3—C2—H2	120.00	C19—C20—H20B	111.00
C2—C3—H3	120.00	H20A—C20—H20B	109.00
C4—C3—H3	120.00		

C16—N1—C17—C18	162.8 (2)	C8—C9—C10—C11	−14.0 (3)
C17—N1—C16—C14	67.5 (2)	C8—C9—C10—C15	164.78 (18)
C20—N1—C16—C14	−172.2 (2)	C15—C10—C11—C12	−0.7 (3)
C17—N1—C20—C19	−34.8 (3)	C11—C10—C15—C14	0.7 (3)
C20—N1—C17—C18	37.6 (3)	C9—C10—C11—C12	178.07 (19)
C16—N1—C20—C19	−159.6 (2)	C9—C10—C15—C14	−178.13 (18)
C6—C1—C2—C3	1.4 (3)	C10—C11—C12—C13	−0.6 (3)
C2—C1—C6—C5	−2.1 (3)	C11—C12—C13—O2	−178.20 (18)
C2—C1—C6—C7	177.4 (2)	C11—C12—C13—C14	1.9 (3)
C1—C2—C3—C4	0.5 (4)	C12—C13—C14—C15	−1.9 (3)
C2—C3—C4—C5	−1.6 (4)	C12—C13—C14—C16	176.13 (19)
C3—C4—C5—C6	0.8 (3)	O2—C13—C14—C15	178.24 (18)
C4—C5—C6—C7	−178.5 (2)	O2—C13—C14—C16	−3.7 (3)
C4—C5—C6—C1	1.0 (3)	C16—C14—C15—C10	−177.39 (19)
C5—C6—C7—C8	15.6 (3)	C13—C14—C15—C10	0.6 (3)
C1—C6—C7—C8	−163.9 (2)	C13—C14—C16—N1	42.4 (3)
C6—C7—C8—C9	178.1 (2)	C15—C14—C16—N1	−139.68 (19)
C7—C8—C9—C10	−174.3 (2)	N1—C17—C18—C19	−25.5 (3)
C7—C8—C9—O1	4.3 (3)	C17—C18—C19—C20	4.3 (3)
O1—C9—C10—C15	−13.8 (3)	C18—C19—C20—N1	18.3 (3)
O1—C9—C10—C11	167.5 (2)		

Hydrogen-bond geometry (Å, º)

Cg3 is the centroid of the C10–C15 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H1*O*···N1	0.85 (3)	1.85 (3)	2.633 (2)	154 (3)
C5—H5···*Cg*3^{i}	0.93	2.99	3.685 (2)	132

Symmetry code: (i) *x*+1/2, −*y*+3/2, −*z*.