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2-Dipentylamino-4-(4-methoxybenzylidene)-1-phenyl-1*H*-imidazol-5(4*H*)-one

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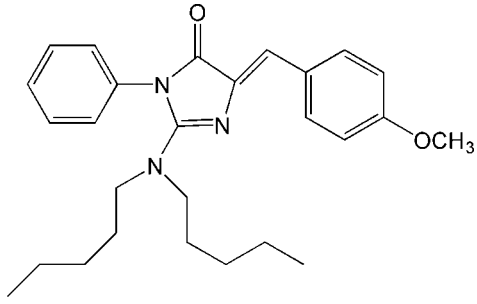
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.063; wR factor = 0.183; data-to-parameter ratio = 14.4.

In the title compound, $C_{27}H_{35}N_3O_2$, one of the pentyl side chains is ordered and the other is highly disordered [the occupancies for the major and minor components are 0.52 (1) and 0.48 (1), respectively]. The dihedral angles between the mean planes of the central C_3N_2 ring and the pendant phenyl and methoxybenzene rings are 88.30 (17) and 9.08 (17)°, respectively. A weak intramolecular C—H···N interaction may help to establish the near planarity of the central and methoxybenzene rings.

Related literature

For a related structure, see: Sun *et al.* (2006). For the synthesis, see: Ding *et al.* (2001).



Experimental

Crystal data

$C_{27}H_{35}N_3O_2$
M_r = 433.58
Triclinic, $P\overline{1}$
a = 9.4091 (8) Å
b = 11.4405 (9) Å
c = 11.9354 (10) Å
α = 90.080 (2)°
β = 94.746 (2)°
γ = 102.044 (2)°
V = 1251.96 (18) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 292 (2) K
0.20 × 0.10 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: none
10980 measured reflections
4871 independent reflections
1734 reflections with $I > 2\sigma(I)$
R_{int} = 0.085

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.183
S = 0.82
4871 reflections
339 parameters
83 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···N1	0.93	2.39	3.037 (4)	127

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); 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: HB2457).

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Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sun, S.-F., Ma, R.-M. & Ng, S. W. (2006). *Acta Cryst.* E**62**, o2090–o2091.

  doi:10.1107/S1600536807030668

supplementary materials

Acta Cryst. (2007). E**63**, o3336 [**doi:10.1107/S1600536807030668**]

2-Dipentylamino-4-(4-methoxybenzylidene)-1-phenyl-1*H*-imidazol-5(4*H*)-one

R. Ma, Z.-Y. Song, Y. Liu, Y.-Q. Bai and F. Bao

Experimental

The compound was synthesized according to a reported procedure (Ding *et al.*, 2001) and yellow blocks of (I) were grown from a dichloromethane/ diethyl ether solution (1:1 *v*/*v*) in about 75% yield. Analysis calculated for $C_{27}H_{35}N_3O_2$: C 74.79, H 8.14, N 9.69%; found: C 74.85, H 8.36, N 9.79%.

Refinement

It is analogous to the examples (Sun *et al.*, 2006), the pentyl chain (C18 to C12) is disordered over two positions; the occupancy factors refined to 0.52 (1):0.48 (1). The pairs of 1,2-related and 1,3- related distances were restrained to be equal within 0.01 Å. The H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Figures

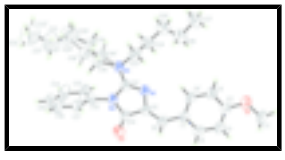


Fig. 1. The molecular structure of (I) with displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radius.

2-Dipentylamino-4-(4-methoxybenzylidene)-1-phenyl-1*H*-imidazol-5(4*H*)-one

Crystal data

$C_{27}H_{35}N_3O_2$	$Z = 2$
$M_r = 433.58$	$F_{000} = 468$
Triclinic, $P\overline{1}$	$D_x = 1.150$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.4091$ (8) Å	Cell parameters from 1232 reflections
$b = 11.4405$ (9) Å	$\theta = 2.6$–$19.1°$
$c = 11.9354$ (10) Å	$\mu = 0.07$ mm^{-1}
$\alpha = 90.080$ (2)°	$T = 292$ (2) K
$\beta = 94.746$ (2)°	Block, yellow
$\gamma = 102.044$ (2)°	0.20 × 0.10 × 0.10 mm
$V = 1251.96$ (18) Å^3	

Data collection

Bruker SMART CCD diffractometer	1734 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.085$
Monochromator: graphite	$\theta_{max} = 26.0^{o}$
$T = 292(2)$ K	$\theta_{min} = 1.7^{o}$
ω scans	$h = -11 \rightarrow 11$
Absorption correction: none	$k = -14 \rightarrow 14$
10980 measured reflections	$l = -14 \rightarrow 14$
4871 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.063$	H-atom parameters constrained
$wR(F^2) = 0.183$	$w = 1/[\sigma^2(F_o^2) + (0.0792P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.82$	$(\Delta/\sigma)_{max} = 0.001$
4871 reflections	$\Delta\rho_{max} = 0.19$ e Å^{-3}
339 parameters	$\Delta\rho_{min} = -0.16$ e Å^{-3}
83 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 $F^2 > 2$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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.3373 (4)	−0.0641 (3)	0.0797 (3)	0.1419 (15)	
H1A	0.4238	−0.0957	0.0775	0.213*	
H1B	0.2829	−0.0752	0.0075	0.213*	
H1C	0.2784	−0.1050	0.1354	0.213*	
C2	0.4595 (4)	0.0944 (3)	0.2069 (3)	0.0871 (9)	

C3	0.5044 (4)	0.0181 (3)	0.2825 (3)	0.0984 (10)	
H3	0.4800	−0.0639	0.2682	0.118*	
C4	0.4948 (3)	0.2159 (3)	0.2300 (3)	0.0904 (9)	
H4	0.4625	0.2683	0.1792	0.108*	
C5	0.5858 (4)	0.0625 (3)	0.3799 (3)	0.0947 (10)	
H5	0.6155	0.0090	0.4308	0.114*	
C6	0.5773 (3)	0.2601 (2)	0.3273 (3)	0.0832 (9)	
H6	0.6012	0.3422	0.3410	0.100*	
C7	0.6254 (3)	0.1840 (2)	0.4055 (2)	0.0731 (8)	
C8	0.7086 (3)	0.2258 (3)	0.5116 (2)	0.0807 (8)	
H8	0.7259	0.1663	0.5607	0.097*	
C9	0.7640 (3)	0.3391 (3)	0.5486 (2)	0.0752 (8)	
C10	0.8344 (3)	0.3676 (3)	0.6628 (3)	0.0859 (9)	
C11	0.8180 (3)	0.5311 (3)	0.5639 (2)	0.0794 (8)	
C12	0.9303 (4)	0.5560 (2)	0.7692 (2)	0.0768 (8)	
C13	0.8467 (4)	0.5797 (3)	0.8493 (3)	0.1260 (14)	
H13	0.7455	0.5582	0.8379	0.151*	
C14	0.9134 (6)	0.6367 (4)	0.9495 (3)	0.1468 (18)	
H14	0.8568	0.6538	1.0052	0.176*	
C15	1.0587 (7)	0.6665 (3)	0.9650 (3)	0.1258 (15)	
H15	1.1035	0.7024	1.0325	0.151*	
C16	1.1403 (5)	0.6449 (3)	0.8832 (4)	0.1293 (14)	
H16	1.2412	0.6694	0.8933	0.155*	
C17	1.0779 (4)	0.5880 (3)	0.7863 (3)	0.1041 (11)	
H17	1.1359	0.5708	0.7317	0.125*	
C18'	0.8293 (7)	0.7435 (5)	0.6198 (5)	0.087 (2)	0.48
H18C	0.8159	0.7106	0.6939	0.104*	0.48
H18D	0.7496	0.7828	0.5982	0.104*	0.48
C19'	0.9726 (10)	0.8314 (6)	0.6210 (8)	0.125 (3)	0.48
H19C	1.0468	0.7937	0.6578	0.150*	0.48
H19D	0.9954	0.8440	0.5436	0.150*	0.48
C20'	0.9882 (14)	0.9510 (7)	0.6752 (8)	0.138 (4)	0.48
H20C	1.0740	1.0027	0.6492	0.165*	0.48
H20D	0.9047	0.9834	0.6476	0.165*	0.48
C21'	1.0005 (15)	0.9595 (9)	0.7999 (6)	0.179 (6)	0.48
H21C	1.0571	0.9026	0.8288	0.215*	0.48
H21D	0.9035	0.9350	0.8251	0.215*	0.48
C22'	1.0690 (16)	1.0806 (11)	0.8523 (10)	0.127 (5)	0.48
H22D	1.0833	1.0734	0.9324	0.191*	0.48
H22E	1.0059	1.1352	0.8350	0.191*	0.48
H22F	1.1614	1.1100	0.8228	0.191*	0.48
C18	0.9372 (8)	0.7502 (5)	0.5874 (6)	0.098 (2)	0.52
H18A	0.9942	0.7232	0.6497	0.118*	0.52
H18B	1.0036	0.7828	0.5318	0.118*	0.52
C19	0.8732 (10)	0.8431 (6)	0.6270 (8)	0.123 (3)	0.52
H19A	0.8397	0.8795	0.5592	0.148*	0.52
H19B	0.7857	0.8015	0.6590	0.148*	0.52
C20	0.9297 (13)	0.9400 (13)	0.7014 (16)	0.240 (10)	0.52
H20A	0.9033	1.0073	0.6617	0.288*	0.52

H20B	0.8665	0.9254	0.7623	0.288*	0.52
C21	1.0651 (13)	0.9887 (14)	0.7559 (12)	0.208 (6)	0.52
H21A	1.1263	1.0165	0.6957	0.249*	0.52
H21B	1.0999	0.9205	0.7870	0.249*	0.52
C22	1.108 (2)	1.0790 (17)	0.8408 (15)	0.242 (10)	0.52
H22A	1.1578	1.1512	0.8086	0.363*	0.52
H22B	1.1710	1.0534	0.8985	0.363*	0.52
H22C	1.0224	1.0937	0.8729	0.363*	0.52
C23	0.7827 (4)	0.6700 (3)	0.4173 (3)	0.1040 (11)	
H23A	0.8301	0.7500	0.3974	0.125*	
H23B	0.8116	0.6138	0.3674	0.125*	
C24	0.6236 (4)	0.6580 (3)	0.4021 (3)	0.1162 (12)	
H24A	0.5943	0.7109	0.4553	0.139*	
H24B	0.5764	0.5767	0.4180	0.139*	
C25	0.5719 (4)	0.6892 (4)	0.2796 (3)	0.1317 (13)	
H25A	0.4689	0.6902	0.2780	0.158*	
H25B	0.6225	0.7701	0.2653	0.158*	
C26	0.5905 (5)	0.6148 (4)	0.1874 (4)	0.1422 (14)	
H26A	0.5425	0.5329	0.2005	0.171*	
H26B	0.6937	0.6168	0.1839	0.171*	
C27	0.5287 (5)	0.6542 (4)	0.0760 (3)	0.1611 (17)	
H27A	0.4270	0.6538	0.0796	0.242*	
H27B	0.5400	0.6004	0.0173	0.242*	
H27C	0.5798	0.7335	0.0606	0.242*	
N1	0.7605 (3)	0.4446 (2)	0.49258 (18)	0.0801 (7)	
N2	0.8658 (3)	0.4919 (2)	0.66852 (19)	0.0875 (7)	
N3	0.8318 (3)	0.6467 (2)	0.5371 (2)	0.0950 (8)	
O1	0.3769 (3)	0.06040 (19)	0.10780 (19)	0.1136 (8)	
O2	0.8609 (3)	0.30362 (19)	0.73927 (19)	0.1186 (8)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.166 (4)	0.101 (3)	0.138 (3)	−0.005 (3)	−0.017 (3)	−0.050 (2)
C2	0.091 (2)	0.080 (2)	0.087 (2)	0.0093 (19)	0.0058 (19)	−0.0139 (19)
C3	0.111 (3)	0.070 (2)	0.110 (3)	0.0121 (19)	0.002 (2)	−0.021 (2)
C4	0.107 (3)	0.081 (2)	0.079 (2)	0.0159 (18)	−0.0001 (19)	−0.0028 (16)
C5	0.111 (3)	0.069 (2)	0.105 (3)	0.0264 (18)	0.000 (2)	−0.0029 (17)
C6	0.101 (2)	0.0652 (18)	0.079 (2)	0.0088 (17)	0.0034 (18)	−0.0037 (16)
C7	0.078 (2)	0.0677 (18)	0.074 (2)	0.0152 (16)	0.0118 (16)	−0.0046 (15)
C8	0.095 (2)	0.076 (2)	0.0747 (19)	0.0267 (17)	0.0086 (17)	0.0047 (15)
C9	0.085 (2)	0.074 (2)	0.0669 (18)	0.0194 (16)	0.0024 (16)	−0.0043 (15)
C10	0.103 (2)	0.080 (2)	0.073 (2)	0.0230 (19)	−0.0073 (18)	−0.0016 (17)
C11	0.102 (2)	0.070 (2)	0.0651 (19)	0.0179 (17)	−0.0036 (17)	−0.0034 (16)
C12	0.080 (2)	0.083 (2)	0.0642 (19)	0.0133 (18)	−0.0056 (17)	−0.0074 (15)
C13	0.098 (3)	0.143 (3)	0.128 (3)	−0.005 (2)	0.032 (3)	−0.053 (3)
C14	0.182 (5)	0.133 (3)	0.109 (3)	−0.027 (3)	0.066 (3)	−0.044 (3)
C15	0.174 (5)	0.110 (3)	0.071 (3)	−0.011 (3)	−0.018 (3)	−0.005 (2)

C16	0.115 (3)	0.141 (3)	0.123 (4)	0.021 (3)	−0.028 (3)	−0.028 (3)
C17	0.091 (3)	0.113 (3)	0.104 (3)	0.016 (2)	−0.002 (2)	−0.030 (2)
C18'	0.096 (5)	0.085 (5)	0.083 (4)	0.027 (4)	0.006 (4)	−0.003 (4)
C19'	0.132 (7)	0.102 (6)	0.139 (7)	0.024 (6)	0.000 (6)	−0.019 (5)
C20'	0.140 (7)	0.104 (6)	0.147 (7)	−0.014 (5)	−0.015 (6)	−0.067 (5)
C21'	0.149 (10)	0.233 (14)	0.144 (11)	0.007 (10)	0.032 (9)	0.084 (11)
C22'	0.146 (9)	0.113 (8)	0.106 (7)	0.003 (7)	−0.023 (6)	−0.074 (7)
C18	0.118 (6)	0.084 (4)	0.085 (4)	0.005 (4)	0.006 (4)	−0.008 (4)
C19	0.149 (7)	0.081 (5)	0.133 (6)	0.008 (5)	0.021 (5)	−0.049 (4)
C20	0.209 (12)	0.205 (13)	0.206 (13)	0.041 (8)	0.050 (9)	−0.004 (9)
C21	0.229 (10)	0.221 (10)	0.167 (9)	0.020 (8)	0.049 (8)	−0.038 (8)
C22	0.228 (16)	0.228 (15)	0.253 (16)	−0.017 (11)	0.079 (12)	0.059 (12)
C23	0.129 (3)	0.075 (2)	0.106 (3)	0.016 (2)	0.016 (2)	0.0037 (17)
C24	0.108 (3)	0.117 (3)	0.128 (3)	0.035 (2)	0.008 (3)	0.005 (2)
C25	0.130 (3)	0.153 (4)	0.119 (3)	0.050 (3)	−0.003 (3)	0.021 (3)
C26	0.168 (4)	0.136 (3)	0.123 (3)	0.041 (3)	−0.012 (3)	−0.014 (3)
C27	0.207 (5)	0.170 (4)	0.098 (3)	0.040 (3)	−0.040 (3)	0.008 (3)
N1	0.1053 (19)	0.0673 (15)	0.0648 (14)	0.0161 (13)	−0.0039 (13)	−0.0020 (13)
N2	0.113 (2)	0.0755 (17)	0.0702 (16)	0.0211 (14)	−0.0194 (14)	−0.0090 (13)
N3	0.136 (2)	0.0739 (18)	0.0695 (17)	0.0192 (16)	−0.0171 (15)	−0.0067 (13)
O1	0.1251 (19)	0.1029 (17)	0.1018 (17)	0.0084 (14)	−0.0134 (14)	−0.0250 (13)
O2	0.169 (2)	0.0942 (16)	0.0889 (16)	0.0336 (15)	−0.0292 (15)	0.0069 (13)

Geometric parameters (Å, °)

C1—O1	1.427 (3)	C19'—H19D	0.9700
C1—H1A	0.9600	C20'—C21'	1.485 (8)
C1—H1B	0.9600	C20'—H20C	0.9700
C1—H1C	0.9600	C20'—H20D	0.9700
C2—C3	1.359 (4)	C21'—C22'	1.511 (8)
C2—O1	1.370 (3)	C21'—H21C	0.9700
C2—C4	1.382 (4)	C21'—H21D	0.9700
C3—C5	1.373 (4)	C22'—H22D	0.9600
C3—H3	0.9300	C22'—H22E	0.9600
C4—C6	1.376 (4)	C22'—H22F	0.9600
C4—H4	0.9300	C18—C19	1.424 (7)
C5—C7	1.389 (4)	C18—N3	1.469 (6)
C5—H5	0.9300	C18—H18A	0.9700
C6—C7	1.389 (4)	C18—H18B	0.9700
C6—H6	0.9300	C19—C20	1.404 (6)
C7—C8	1.457 (4)	C19—H19A	0.9700
C8—C9	1.351 (3)	C19—H19B	0.9700
C8—H8	0.9300	C20—C21	1.387 (8)
C9—N1	1.385 (3)	C20—H20A	0.9700
C9—C10	1.470 (4)	C20—H20B	0.9700
C10—O2	1.213 (3)	C21—C22	1.419 (8)
C10—N2	1.392 (3)	C21—H21A	0.9700
C11—N1	1.302 (3)	C21—H21B	0.9700
C11—N3	1.343 (3)	C22—H22A	0.9600

C11—N2	1.398 (3)	C22—H22B	0.9600
C12—C13	1.348 (4)	C22—H22C	0.9600
C12—C17	1.359 (4)	C23—C24	1.471 (4)
C12—N2	1.429 (3)	C23—N3	1.508 (4)
C13—C14	1.398 (5)	C23—H23A	0.9700
C13—H13	0.9300	C23—H23B	0.9700
C14—C15	1.336 (5)	C24—C25	1.569 (5)
C14—H14	0.9300	C24—H24A	0.9700
C15—C16	1.344 (5)	C24—H24B	0.9700
C15—H15	0.9300	C25—C26	1.434 (5)
C16—C17	1.353 (4)	C25—H25A	0.9700
C16—H16	0.9300	C25—H25B	0.9700
C17—H17	0.9300	C26—C27	1.515 (5)
C18'—N3	1.488 (6)	C26—H26A	0.9700
C18'—C19'	1.503 (7)	C26—H26B	0.9700
C18'—H18C	0.9700	C27—H27A	0.9600
C18'—H18D	0.9700	C27—H27B	0.9600
C19'—C20'	1.487 (7)	C27—H27C	0.9600
C19'—H19C	0.9700		
O1—C1—H1A	109.5	C20'—C21'—H21D	108.1
O1—C1—H1B	109.5	C22'—C21'—H21D	108.1
H1A—C1—H1B	109.5	H21C—C21'—H21D	107.3
O1—C1—H1C	109.5	C21'—C22'—H22D	109.5
H1A—C1—H1C	109.5	C21'—C22'—H22E	109.5
H1B—C1—H1C	109.5	H22D—C22'—H22E	109.5
C3—C2—O1	124.9 (3)	C21'—C22'—H22F	109.5
C3—C2—C4	119.4 (3)	H22D—C22'—H22F	109.5
O1—C2—C4	115.7 (3)	H22E—C22'—H22F	109.5
C2—C3—C5	119.8 (3)	C19—C18—N3	114.4 (6)
C2—C3—H3	120.1	C19—C18—H18A	108.7
C5—C3—H3	120.1	N3—C18—H18A	108.7
C6—C4—C2	120.6 (3)	C19—C18—H18B	108.7
C6—C4—H4	119.7	N3—C18—H18B	108.7
C2—C4—H4	119.7	H18A—C18—H18B	107.6
C3—C5—C7	122.6 (3)	C20—C19—C18	131.3 (7)
C3—C5—H5	118.7	C20—C19—H19A	104.4
C7—C5—H5	118.7	C18—C19—H19A	104.4
C4—C6—C7	121.1 (3)	C20—C19—H19B	104.4
C4—C6—H6	119.5	C18—C19—H19B	104.4
C7—C6—H6	119.5	H19A—C19—H19B	105.6
C6—C7—C5	116.5 (3)	C21—C20—C19	135.7 (9)
C6—C7—C8	123.3 (3)	C21—C20—H20A	103.3
C5—C7—C8	120.2 (3)	C19—C20—H20A	103.3
C9—C8—C7	128.9 (3)	C21—C20—H20B	103.3
C9—C8—H8	115.5	C19—C20—H20B	103.3
C7—C8—H8	115.5	H20A—C20—H20B	105.2
C8—C9—N1	128.3 (3)	C20—C21—C22	131.1 (12)
C8—C9—C10	122.5 (3)	C20—C21—H21A	104.5
N1—C9—C10	109.1 (2)	C22—C21—H21A	104.5

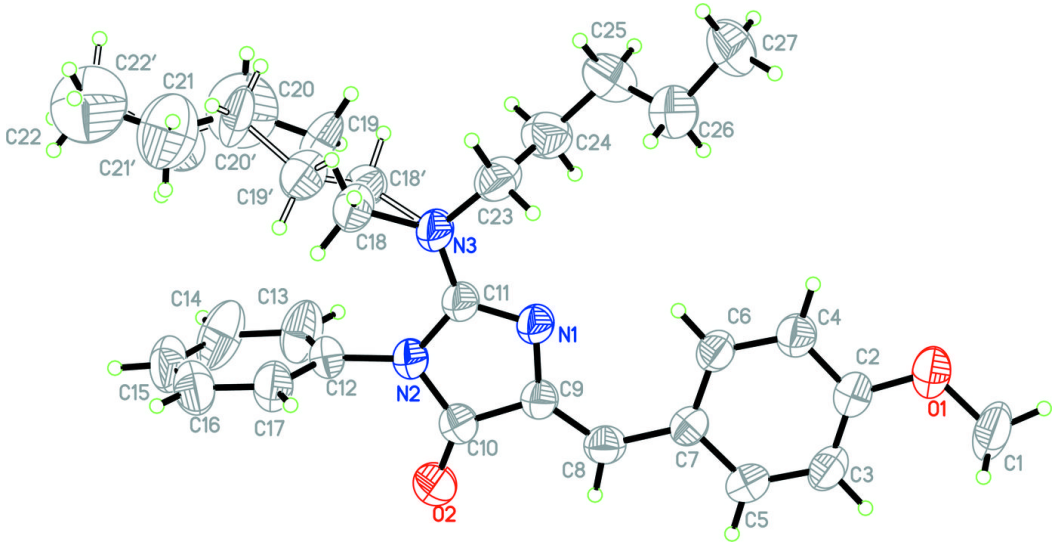
O2—C10—N2	124.6 (3)	C20—C21—H21B	104.5
O2—C10—C9	131.3 (3)	C22—C21—H21B	104.5
N2—C10—C9	104.0 (3)	H21A—C21—H21B	105.6
N1—C11—N3	122.3 (3)	C24—C23—N3	111.1 (3)
N1—C11—N2	113.7 (2)	C24—C23—H23A	109.4
N3—C11—N2	124.0 (3)	N3—C23—H23A	109.4
C13—C12—C17	120.0 (3)	C24—C23—H23B	109.4
C13—C12—N2	120.7 (3)	N3—C23—H23B	109.4
C17—C12—N2	119.2 (3)	H23A—C23—H23B	108.0
C12—C13—C14	119.4 (4)	C23—C24—C25	111.7 (3)
C12—C13—H13	120.3	C23—C24—H24A	109.3
C14—C13—H13	120.3	C25—C24—H24A	109.3
C15—C14—C13	119.7 (4)	C23—C24—H24B	109.3
C15—C14—H14	120.1	C25—C24—H24B	109.3
C13—C14—H14	120.1	H24A—C24—H24B	107.9
C14—C15—C16	120.1 (4)	C26—C25—C24	119.1 (3)
C14—C15—H15	120.0	C26—C25—H25A	107.5
C16—C15—H15	120.0	C24—C25—H25A	107.5
C15—C16—C17	121.0 (4)	C26—C25—H25B	107.5
C15—C16—H16	119.5	C24—C25—H25B	107.5
C17—C16—H16	119.5	H25A—C25—H25B	107.0
C16—C17—C12	119.7 (3)	C25—C26—C27	112.2 (4)
C16—C17—H17	120.1	C25—C26—H26A	109.2
C12—C17—H17	120.1	C27—C26—H26A	109.2
N3—C18'—C19'	107.7 (6)	C25—C26—H26B	109.2
N3—C18'—H18C	110.2	C27—C26—H26B	109.2
C19'—C18'—H18C	110.2	H26A—C26—H26B	107.9
N3—C18'—H18D	110.2	C26—C27—H27A	109.5
C19'—C18'—H18D	110.2	C26—C27—H27B	109.5
H18C—C18'—H18D	108.5	H27A—C27—H27B	109.5
C20'—C19'—C18'	119.3 (8)	C26—C27—H27C	109.5
C20'—C19'—H19C	107.5	H27A—C27—H27C	109.5
C18'—C19'—H19C	107.5	H27B—C27—H27C	109.5
C20'—C19'—H19D	107.5	C11—N1—C9	106.4 (2)
C18'—C19'—H19D	107.5	C10—N2—C11	106.7 (2)
H19C—C19'—H19D	107.0	C10—N2—C12	121.7 (2)
C21'—C20'—C19'	118.4 (8)	C11—N2—C12	131.5 (2)
C21'—C20'—H20C	107.7	C11—N3—C18	128.1 (4)
C19'—C20'—H20C	107.7	C11—N3—C18'	123.8 (3)
C21'—C20'—H20D	107.7	C18—N3—C18'	43.8 (3)
C19'—C20'—H20D	107.7	C11—N3—C23	115.7 (2)
H20C—C20'—H20D	107.1	C18—N3—C23	111.2 (3)
C20'—C21'—C22'	116.6 (9)	C18'—N3—C23	115.3 (3)
C20'—C21'—H21C	108.1	C2—O1—C1	118.0 (3)
C22'—C21'—H21C	108.1		
O1—C2—C3—C5	−179.3 (3)	C24—C25—C26—C27	177.4 (4)
C4—C2—C3—C5	−0.9 (5)	N3—C11—N1—C9	−179.9 (3)
C3—C2—C4—C6	1.4 (5)	N2—C11—N1—C9	1.3 (3)
O1—C2—C4—C6	179.9 (3)	C8—C9—N1—C11	175.6 (3)

C2—C3—C5—C7	−0.1 (5)	C10—C9—N1—C11	−1.7 (3)
C2—C4—C6—C7	−0.9 (4)	O2—C10—N2—C11	−179.8 (3)
C4—C6—C7—C5	−0.1 (4)	C9—C10—N2—C11	−0.7 (3)
C4—C6—C7—C8	−177.8 (3)	O2—C10—N2—C12	−1.7 (5)
C3—C5—C7—C6	0.6 (4)	C9—C10—N2—C12	177.3 (3)
C3—C5—C7—C8	178.3 (3)	N1—C11—N2—C10	−0.3 (3)
C6—C7—C8—C9	−6.6 (5)	N3—C11—N2—C10	−179.1 (3)
C5—C7—C8—C9	175.8 (3)	N1—C11—N2—C12	−178.1 (3)
C7—C8—C9—N1	−2.8 (5)	N3—C11—N2—C12	3.1 (5)
C7—C8—C9—C10	174.1 (3)	C13—C12—N2—C10	−86.3 (4)
C8—C9—C10—O2	3.0 (5)	C17—C12—N2—C10	90.5 (4)
N1—C9—C10—O2	−179.5 (3)	C13—C12—N2—C11	91.3 (4)
C8—C9—C10—N2	−176.0 (2)	C17—C12—N2—C11	−92.0 (4)
N1—C9—C10—N2	1.5 (3)	N1—C11—N3—C18	−155.0 (4)
C17—C12—C13—C14	−0.2 (5)	N2—C11—N3—C18	23.7 (6)
N2—C12—C13—C14	176.5 (3)	N1—C11—N3—C18'	150.4 (4)
C12—C13—C14—C15	−0.3 (6)	N2—C11—N3—C18'	−30.9 (5)
C13—C14—C15—C16	1.9 (7)	N1—C11—N3—C23	−2.8 (4)
C14—C15—C16—C17	−3.1 (7)	N2—C11—N3—C23	175.9 (3)
C15—C16—C17—C12	2.5 (6)	C19—C18—N3—C11	−125.9 (6)
C13—C12—C17—C16	−0.9 (5)	C19—C18—N3—C18'	−24.2 (6)
N2—C12—C17—C16	−177.6 (3)	C19—C18—N3—C23	80.8 (7)
N3—C18'—C19'—C20'	165.8 (7)	C19'—C18'—N3—C11	119.8 (6)
C18'—C19'—C20'—C21'	74.3 (14)	C19'—C18'—N3—C18	7.8 (6)
C19'—C20'—C21'—C22'	158.6 (11)	C19'—C18'—N3—C23	−87.0 (6)
N3—C18—C19—C20	162.9 (15)	C24—C23—N3—C11	81.5 (3)
C18—C19—C20—C21	7(4)	C24—C23—N3—C18	−121.7 (4)
C19—C20—C21—C22	−171.2 (18)	C24—C23—N3—C18'	−73.9 (4)
N3—C23—C24—C25	176.7 (3)	C3—C2—O1—C1	−1.5 (5)
C23—C24—C25—C26	65.0 (5)	C4—C2—O1—C1	180.0 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···N1	0.93	2.39	3.037 (4)	127

Fig. 1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C12
N2
C9
C16
C17
C10
C8
C7
C3
C1
O2
C5