

## 2-(4-Methoxyphenyl)-1-pentyl-4,5-diphenyl-1*H*-imidazole

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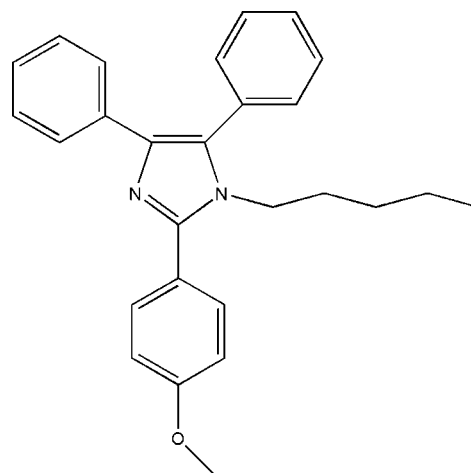
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Key indicators: single-crystal X-ray study;  $T = 93$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.048;  $wR$  factor = 0.132; data-to-parameter ratio = 18.2.

The title compound,  $\text{C}_{27}\text{H}_{28}\text{N}_2\text{O}$ , is a lophine (2,4,5-triphenyl-1*H*-imidazole) derivative with an *n*-pentyl chain on the amine N atom and a 4-methoxy substituent on the benzene ring. The two phenyl and methoxybenzene rings are inclined to the imidazole ring at angles of 25.32 (7), 76.79 (5) and 35.42 (7)°, respectively, while the methoxy substituent lies close to the plane of its benzene ring, with a maximum deviation of 0.126 (3) Å for the methoxy C atom. In the crystal, inversion dimers linked by pairs of  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds generate  $R_2^2(22)$  loops. These dimers are stacked along the *a*-axis direction.

### Related literature

For the non-linear optical and chemiluminescence properties of lophine and its derivatives, see: Santos *et al.* (2001); Radziszewski (1877); Maeda & Hayashi (1969, 1970). For the bioactivity of imidazoles, see: Antolini *et al.* (1999); Evers *et al.* (1998); Laszlo *et al.* (1999); Newman *et al.* (2000); Veisi *et al.* (2012); Wang *et al.* (2002). For related structures, see, for example: Yanover & Kaftory (2009*a,b*); Kison & Opatz (2009); Zhao *et al.* (2012). For representative bond lengths, see: Allen *et al.* (1987) and for hydrogen-bond motifs, see: Bernstein *et al.* (1995).



### Experimental

#### Crystal data

$\text{C}_{27}\text{H}_{28}\text{N}_2\text{O}$   
 $M_r = 396.51$   
 Triclinic,  $P\bar{1}$   
 $a = 9.7214$  (19) Å  
 $b = 10.739$  (1) Å  
 $c = 11.7367$  (10) Å  
 $\alpha = 114.069$  (4)°  
 $\beta = 99.021$  (6)°

$\gamma = 95.425$  (6)°  
 $V = 1087.7$  (3) Å<sup>3</sup>  
 $Z = 2$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.07$  mm<sup>-1</sup>  
 $T = 93$  K  
 $0.47 \times 0.18 \times 0.08$  mm

#### Data collection

Bruker APEXII CCD area-detector diffractometer  
 Absorption correction: multi-scan (SADABS; Bruker, 2011)  
 $T_{\min} = 0.619$ ,  $T_{\max} = 0.746$

15574 measured reflections  
 4968 independent reflections  
 3542 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.043$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.048$   
 $wR(F^2) = 0.132$   
 $S = 1.06$   
 4968 reflections

273 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.21$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.25$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C}15-\text{H}15\cdots\text{O}119^i$	0.95	2.61	3.4393 (19)	146

Symmetry code: (i)  $-x + 2, -y + 2, -z + 2$ .

Data collection: APEX2 (Bruker, 2011); cell refinement: APEX2 and SAINT (Bruker, 2011); data reduction: SAINT (Bruker, 2011); program(s) used to solve structure: SHELXS97 (Sheldrick, 2008) and TITAN2000 (Hunter & Simpson, 1999); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008) and TITAN2000; molecular graphics: SHELXTL (Sheldrick, 2008) and Mercury (Macrae *et al.*, 2008); software used to prepare material for publication: SHELXL97, enCIFer (Allen *et al.*, 2004), PLATON (Spek, 2009) and publCIF (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT6874).

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## supporting information

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**2-(4-Methoxyphenyl)-1-pentyl-4,5-diphenyl-1*H*-imidazole**

**Jim Simpson, Shaaban K. Mohamed, Adel A. Marzouk, Avtandil H. Talybov and Antar A. Abdelhamid**

**S1. Comment**

The chemilumescence properties of lophine, (2,4,5-triphenyl-1*H*-imidazole), and its derivatives have been known since the late 19th century (Radziszewski, 1877) and their non-linear optical (Santos *et al.*, 2001) and related optical properties (Maeda & Hayashi, 1969, 1970) have been extensively investigated. In addition, substituted imidazoles exhibit a wide range of biological activities for example as glucagon receptors (Laszlo *et al.*, 1999), CB1 cannabinoid receptor antagonists (Eyers *et al.*, 1998) and modulators of P-glycoprotein (P-gp)-mediated multi drug resistance (MDR) (Newman *et al.*, 2000). They can also act as both antibacterial (Antolini *et al.*, 1999) and antitumor agents (Wang *et al.*, 2002) or as pesticides (Veisi *et al.*, 2012). As part of our work on the synthesis of imidazole derivatives, we have prepared 2-(4-methoxyphenyl)-1-pentyl-4,5-diphenyl-1*H*-imidazole and report its preparation and structure here.

In the title compound, the lophine (2,4,5-triphenyl-1*H*-imidazole) skeleton (Yanover & Kaftory, 2009*a*) is embellished with a nicely ordered C22—C26 *n*-pentyl substituent on the amine N atom of the imidazole ring and a *p*-methoxy substituent on the C17—C21 benzene ring. The *n*-pentyl chain is almost orthogonal to the imidazole with a meanplane through C22⋯C26 (r.m.s. deviation = 0.047 %Å) that subtends a dihedral angle of 78.91 (7) ° to the plane of the imidazole ring. The two C4⋯C9 and C10⋯C15 phenyl rings are inclined to the imidazole ring at angles of 25.32 (7)°, 76.79 (5)° respectively while the methoxy substituted C17⋯C21 ring makes an angle of 35.42 (7)°. The methoxy substituent lies close to the plane of the C17⋯C21 benzene ring with a maximum deviation of only 0.126 (3) Å for the C119 atom. Bond distances in the structure are normal (Allen *et al.*, 1987) and are comparable to those reported for related structures (Yanover & Kaftory, 2009*a,b*; Kison & Opatz, 2009; Zhao *et al.*, 2012). In the crystal structure the only significant intermolecular contacts are C15—H15⋯O119 hydrogen bonds which form inversion dimers with  $R_2^2(22)$  ring motifs (Bernstein *et al.*, 1995). These dimers are further stacked along the *a* axis (Fig. 2), with alternating molecules arranged in a head to tail fashion (Fig. 3).

**S2. Experimental**

A 50-ml. volumetric flask equipped with a magnetic stirring bar was charged with 25 ml. of dimethyl sulfoxide and 2.4 g (40 mmol) potassium hydroxide. The mixture was stirred at room temperature for 5 minutes, then 3.26 g (10 mmol) 2-(4-methoxyphenyl)-4,5-diphenyl-1*H*-imidazole was added with stirring for a further 45 minutes. To this reaction mixture, 3.02 g. (20 mmol) pentyl bromide was added. After stirring for an additional 45 minutes the mixture was diluted with 20 ml water then extracted with diethyl ether (3x 20 ml). The combined ether layers were dried over calcium chloride and evaporated under slightly reduced pressure. The excess pentyl bromide was removed by distillation at approximately 15 mm, and the residue was crystallized from ethanol yielding 3.35 g (84%) of 2-(4-methoxyphenyl)-1-pentyl-4,5-diphenyl-1*H*-imidazole, m.p. 382–384 K.

### S3. Refinement

All H-atoms bound were refined using a riding model with  $d(\text{C}-\text{H}) = 0.95 \text{ \AA}$ ,  $U_{\text{iso}} = 1.2U_{\text{eq}}(\text{C})$  for aromatic,  $0.99 \text{ \AA}$   $U_{\text{iso}} = 1.2U_{\text{eq}}(\text{C})$  for methylene and  $0.98 \text{ \AA}$ ,  $U_{\text{iso}} = 1.5U_{\text{eq}}(\text{C})$  for  $\text{CH}_3$  H atoms.

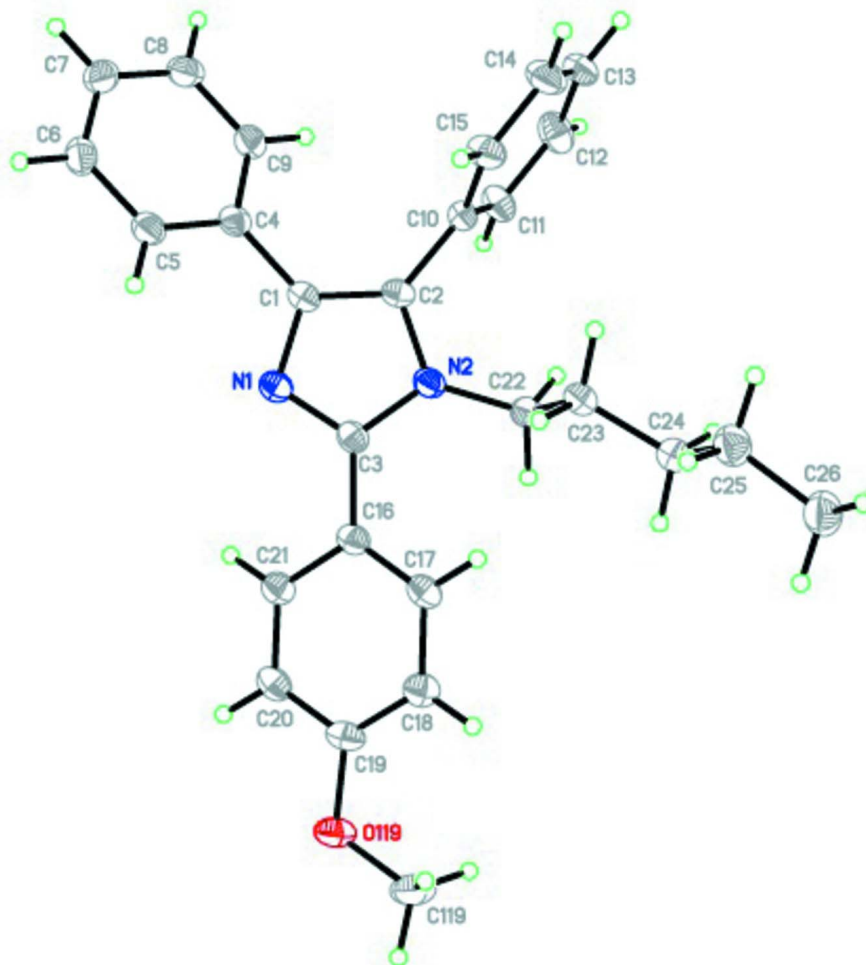
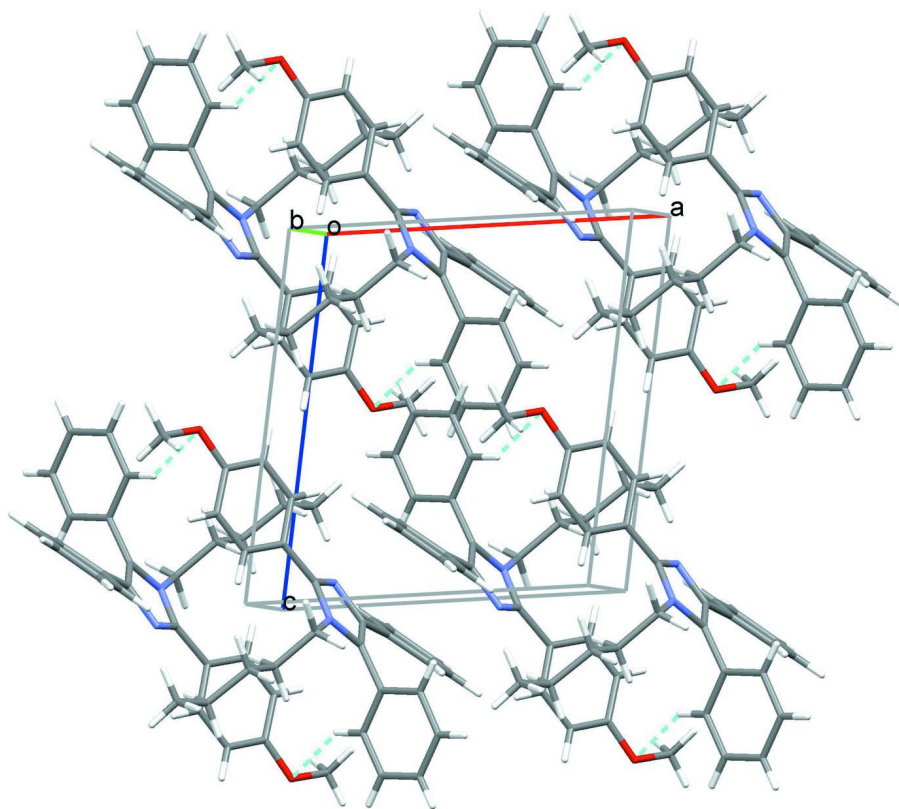


Figure 1

The structure of I with ellipsoids drawn at the 50% probability level.



**Figure 2**

Crystal packing of **I** viewed along *b* showing centrosymmetric dimer formation. Hydrogen bonds are drawn as dashed lines.

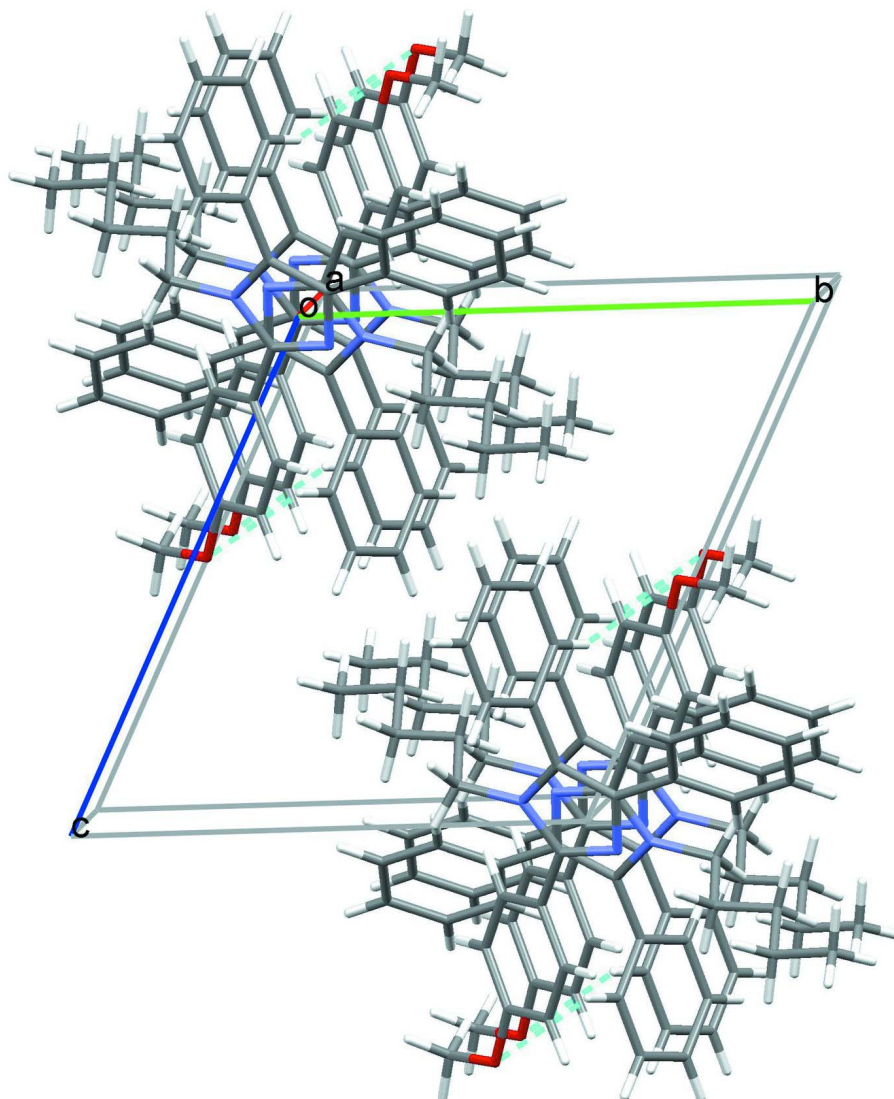


Figure 3

Crystal packing of **I** showing stacks formed along *a*. Hydrogen bonds are drawn as dashed lines.

### 2-(4-Methoxyphenyl)-1-pentyl-4,5-diphenyl-1*H*-imidazole

#### Crystal data

$C_{27}H_{28}N_2O$

$M_r = 396.51$

Triclinic,  $P\bar{1}$

Hall symbol:  $-P\ 1$

$a = 9.7214$  (19) Å

$b = 10.739$  (1) Å

$c = 11.7367$  (10) Å

$\alpha = 114.069$  (4)°

$\beta = 99.021$  (6)°

$\gamma = 95.425$  (6)°

$V = 1087.7$  (3) Å<sup>3</sup>

$Z = 2$

$F(000) = 424$

$D_x = 1.211$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 3238 reflections

$\theta = 2.6$ – $26.1$ °

$\mu = 0.07$  mm<sup>-1</sup>

$T = 93$  K

Rectangular plate, colourless

$0.47 \times 0.18 \times 0.08$  mm

Data collection

Bruker APEXII CCD area-detector  
diffractometer  
Radiation source: fine-focus sealed tube  
Graphite monochromator  
 $\omega$  scans  
Absorption correction: multi-scan  
(SADABS; Bruker, 2011)  
 $T_{\min} = 0.619$ ,  $T_{\max} = 0.746$

15574 measured reflections  
4968 independent reflections  
3542 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.043$   
 $\theta_{\max} = 27.6^\circ$ ,  $\theta_{\min} = 3.1^\circ$   
 $h = -12 \rightarrow 12$   
 $k = -13 \rightarrow 14$   
 $l = -15 \rightarrow 15$

Refinement

Refinement on  $F^2$   
Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.048$   
 $wR(F^2) = 0.132$   
 $S = 1.06$   
4968 reflections  
273 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0663P)^2 + 0.0245P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.21 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.25 \text{ e } \text{\AA}^{-3}$

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.

**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 ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.65447 (14)	1.04609 (14)	0.93573 (12)	0.0209 (3)
C2	0.63626 (14)	0.90460 (14)	0.87092 (12)	0.0208 (3)
N2	0.73101 (12)	0.86376 (11)	0.94408 (10)	0.0214 (3)
C3	0.80178 (14)	0.98139 (14)	1.04912 (13)	0.0206 (3)
N1	0.75725 (12)	1.09265 (12)	1.04654 (10)	0.0218 (3)
C4	0.58701 (15)	1.14575 (14)	0.89992 (12)	0.0213 (3)
C5	0.65877 (16)	1.28159 (15)	0.94687 (13)	0.0252 (3)
H5	0.7490	1.3086	1.0031	0.030*
C6	0.60042 (16)	1.37763 (15)	0.91278 (14)	0.0276 (3)
H6	0.6507	1.4696	0.9454	0.033*
C7	0.46848 (16)	1.33933 (16)	0.83088 (14)	0.0290 (4)
H7	0.4288	1.4045	0.8064	0.035*
C8	0.39535 (17)	1.20596 (16)	0.78529 (14)	0.0283 (4)
H8	0.3045	1.1798	0.7302	0.034*
C9	0.45371 (15)	1.11015 (15)	0.81940 (13)	0.0244 (3)
H9	0.4022	1.0188	0.7875	0.029*

C10	0.54830 (15)	0.80462 (14)	0.74497 (13)	0.0210 (3)
C11	0.42624 (16)	0.71869 (15)	0.73438 (14)	0.0279 (4)
H11	0.3970	0.7226	0.8091	0.033*
C12	0.34667 (17)	0.62676 (16)	0.61431 (15)	0.0334 (4)
H12	0.2637	0.5677	0.6077	0.040*
C13	0.38700 (17)	0.62053 (16)	0.50497 (14)	0.0310 (4)
H13	0.3321	0.5577	0.4233	0.037*
C14	0.50733 (17)	0.70598 (16)	0.51489 (14)	0.0329 (4)
H14	0.5353	0.7026	0.4398	0.040*
C15	0.58783 (16)	0.79690 (15)	0.63386 (13)	0.0280 (4)
H15	0.6713	0.8548	0.6396	0.034*
C16	0.90797 (15)	0.98543 (14)	1.15551 (13)	0.0216 (3)
C17	1.00822 (15)	0.89913 (15)	1.14112 (13)	0.0240 (3)
H17	1.0102	0.8329	1.0579	0.029*
C18	1.10545 (15)	0.90705 (15)	1.24484 (13)	0.0249 (3)
H18	1.1723	0.8462	1.2326	0.030*
C19	1.10445 (15)	1.00433 (15)	1.36650 (13)	0.0243 (3)
O119	1.19783 (10)	1.02238 (11)	1.47489 (9)	0.0288 (3)
C119	1.28969 (17)	0.92355 (17)	1.46185 (15)	0.0351 (4)
H11A	1.2332	0.8303	1.4256	0.053*
H11B	1.3471	0.9442	1.5459	0.053*
H11C	1.3518	0.9283	1.4050	0.053*
C20	1.00777 (15)	1.09470 (15)	1.38280 (13)	0.0255 (3)
H20	1.0087	1.1633	1.4658	0.031*
C21	0.91080 (15)	1.08526 (15)	1.27931 (13)	0.0242 (3)
H21	0.8450	1.1471	1.2918	0.029*
C22	0.75400 (15)	0.72148 (14)	0.90983 (13)	0.0228 (3)
H22A	0.6625	0.6574	0.8669	0.027*
H22B	0.7908	0.7114	0.9886	0.027*
C23	0.85838 (15)	0.68150 (14)	0.82145 (13)	0.0241 (3)
H23A	0.8103	0.6648	0.7344	0.029*
H23B	0.9379	0.7599	0.8518	0.029*
C24	0.91712 (16)	0.55285 (15)	0.81503 (14)	0.0260 (3)
H24A	0.9624	0.5680	0.9024	0.031*
H24B	0.8381	0.4734	0.7814	0.031*
C25	1.02476 (16)	0.51780 (16)	0.73060 (14)	0.0311 (4)
H25A	0.9762	0.4906	0.6411	0.037*
H25B	1.0966	0.6017	0.7571	0.037*
C26	1.09912 (18)	0.40151 (16)	0.73654 (16)	0.0359 (4)
H26A	1.1529	0.4301	0.8237	0.054*
H26B	1.1637	0.3809	0.6775	0.054*
H26C	1.0286	0.3185	0.7122	0.054*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0207 (7)	0.0229 (7)	0.0170 (7)	0.0013 (6)	0.0033 (6)	0.0072 (6)
C2	0.0205 (7)	0.0251 (7)	0.0170 (7)	0.0031 (6)	0.0037 (5)	0.0097 (6)



N2	0.0241 (6)	0.0216 (6)	0.0168 (6)	0.0025 (5)	0.0030 (5)	0.0075 (5)
C3	0.0221 (7)	0.0216 (7)	0.0172 (7)	0.0025 (6)	0.0059 (6)	0.0071 (6)
N1	0.0229 (6)	0.0238 (6)	0.0180 (6)	0.0035 (5)	0.0047 (5)	0.0081 (5)
C4	0.0243 (7)	0.0244 (7)	0.0154 (7)	0.0067 (6)	0.0074 (6)	0.0070 (6)
C5	0.0268 (8)	0.0255 (8)	0.0196 (7)	0.0052 (6)	0.0032 (6)	0.0066 (6)
C6	0.0352 (9)	0.0212 (7)	0.0255 (8)	0.0044 (6)	0.0090 (7)	0.0083 (6)
C7	0.0373 (9)	0.0294 (8)	0.0235 (8)	0.0136 (7)	0.0083 (7)	0.0124 (7)
C8	0.0292 (8)	0.0331 (8)	0.0209 (7)	0.0088 (7)	0.0034 (6)	0.0098 (7)
C9	0.0259 (8)	0.0235 (8)	0.0211 (7)	0.0045 (6)	0.0054 (6)	0.0067 (6)
C10	0.0229 (7)	0.0201 (7)	0.0182 (7)	0.0053 (6)	0.0031 (6)	0.0067 (6)
C11	0.0296 (8)	0.0271 (8)	0.0222 (7)	0.0021 (6)	0.0084 (6)	0.0056 (6)
C12	0.0265 (8)	0.0299 (8)	0.0327 (9)	-0.0018 (7)	0.0048 (7)	0.0047 (7)
C13	0.0321 (9)	0.0293 (8)	0.0208 (7)	0.0055 (7)	-0.0042 (6)	0.0038 (6)
C14	0.0405 (9)	0.0363 (9)	0.0184 (7)	0.0037 (7)	0.0042 (7)	0.0096 (7)
C15	0.0292 (8)	0.0305 (8)	0.0223 (7)	-0.0008 (6)	0.0031 (6)	0.0116 (7)
C16	0.0223 (7)	0.0227 (7)	0.0187 (7)	0.0009 (6)	0.0033 (6)	0.0089 (6)
C17	0.0254 (8)	0.0257 (8)	0.0177 (7)	0.0023 (6)	0.0049 (6)	0.0065 (6)
C18	0.0225 (8)	0.0286 (8)	0.0238 (7)	0.0046 (6)	0.0053 (6)	0.0114 (6)
C19	0.0217 (7)	0.0316 (8)	0.0189 (7)	-0.0009 (6)	0.0008 (6)	0.0128 (6)
O119	0.0271 (6)	0.0383 (6)	0.0204 (5)	0.0066 (5)	0.0007 (4)	0.0135 (5)
C119	0.0310 (9)	0.0456 (10)	0.0290 (8)	0.0105 (8)	-0.0007 (7)	0.0180 (8)
C20	0.0277 (8)	0.0267 (8)	0.0185 (7)	0.0024 (6)	0.0055 (6)	0.0064 (6)
C21	0.0243 (8)	0.0255 (7)	0.0210 (7)	0.0040 (6)	0.0048 (6)	0.0084 (6)
C22	0.0249 (7)	0.0206 (7)	0.0214 (7)	0.0022 (6)	0.0013 (6)	0.0092 (6)
C23	0.0268 (8)	0.0234 (7)	0.0188 (7)	0.0033 (6)	0.0026 (6)	0.0068 (6)
C24	0.0276 (8)	0.0263 (8)	0.0227 (7)	0.0054 (6)	0.0037 (6)	0.0095 (6)
C25	0.0320 (9)	0.0300 (8)	0.0292 (8)	0.0073 (7)	0.0080 (7)	0.0097 (7)
C26	0.0339 (9)	0.0317 (9)	0.0369 (9)	0.0088 (7)	0.0076 (7)	0.0091 (7)

*Geometric parameters (Å, °)*

C1—C2	1.3721 (19)	C16—C17	1.390 (2)
C1—N1	1.3811 (17)	C16—C21	1.4045 (19)
C1—C4	1.4716 (19)	C17—C18	1.3864 (19)
C2—N2	1.3833 (17)	C17—H17	0.9500
C2—C10	1.4848 (18)	C18—C19	1.386 (2)
N2—C3	1.3742 (17)	C18—H18	0.9500
N2—C22	1.4622 (17)	C19—O119	1.3724 (16)
C3—N1	1.3188 (17)	C19—C20	1.393 (2)
C3—C16	1.4730 (19)	O119—C119	1.4272 (18)
C4—C9	1.3950 (19)	C119—H11A	0.9800
C4—C5	1.396 (2)	C119—H11B	0.9800
C5—C6	1.386 (2)	C119—H11C	0.9800
C5—H5	0.9500	C20—C21	1.3772 (19)
C6—C7	1.389 (2)	C20—H20	0.9500
C6—H6	0.9500	C21—H21	0.9500
C7—C8	1.381 (2)	C22—C23	1.529 (2)
C7—H7	0.9500	C22—H22A	0.9900

C8—C9	1.384 (2)	C22—H22B	0.9900
C8—H8	0.9500	C23—C24	1.5225 (19)
C9—H9	0.9500	C23—H23A	0.9900
C10—C15	1.389 (2)	C23—H23B	0.9900
C10—C11	1.389 (2)	C24—C25	1.521 (2)
C11—C12	1.392 (2)	C24—H24A	0.9900
C11—H11	0.9500	C24—H24B	0.9900
C12—C13	1.378 (2)	C25—C26	1.521 (2)
C12—H12	0.9500	C25—H25A	0.9900
C13—C14	1.375 (2)	C25—H25B	0.9900
C13—H13	0.9500	C26—H26A	0.9800
C14—C15	1.384 (2)	C26—H26B	0.9800
C14—H14	0.9500	C26—H26C	0.9800
C15—H15	0.9500		
C2—C1—N1	110.31 (12)	C18—C17—C16	121.84 (13)
C2—C1—C4	129.52 (12)	C18—C17—H17	119.1
N1—C1—C4	120.10 (12)	C16—C17—H17	119.1
C1—C2—N2	105.42 (11)	C19—C18—C17	119.52 (14)
C1—C2—C10	132.42 (13)	C19—C18—H18	120.2
N2—C2—C10	121.98 (12)	C17—C18—H18	120.2
C3—N2—C2	107.27 (11)	O119—C19—C18	124.04 (13)
C3—N2—C22	127.52 (12)	O119—C19—C20	116.28 (12)
C2—N2—C22	125.14 (11)	C18—C19—C20	119.63 (13)
N1—C3—N2	111.01 (12)	C19—O119—C119	117.07 (11)
N1—C3—C16	123.28 (12)	O119—C119—H11A	109.5
N2—C3—C16	125.62 (12)	O119—C119—H11B	109.5
C3—N1—C1	105.98 (11)	H11A—C119—H11B	109.5
C9—C4—C5	118.02 (13)	O119—C119—H11C	109.5
C9—C4—C1	122.72 (13)	H11A—C119—H11C	109.5
C5—C4—C1	119.25 (13)	H11B—C119—H11C	109.5
C6—C5—C4	121.02 (13)	C21—C20—C19	120.41 (13)
C6—C5—H5	119.5	C21—C20—H20	119.8
C4—C5—H5	119.5	C19—C20—H20	119.8
C5—C6—C7	119.98 (14)	C20—C21—C16	120.87 (14)
C5—C6—H6	120.0	C20—C21—H21	119.6
C7—C6—H6	120.0	C16—C21—H21	119.6
C8—C7—C6	119.63 (14)	N2—C22—C23	112.03 (12)
C8—C7—H7	120.2	N2—C22—H22A	109.2
C6—C7—H7	120.2	C23—C22—H22A	109.2
C7—C8—C9	120.34 (14)	N2—C22—H22B	109.2
C7—C8—H8	119.8	C23—C22—H22B	109.2
C9—C8—H8	119.8	H22A—C22—H22B	107.9
C8—C9—C4	121.00 (14)	C24—C23—C22	113.10 (12)
C8—C9—H9	119.5	C24—C23—H23A	109.0
C4—C9—H9	119.5	C22—C23—H23A	109.0
C15—C10—C11	118.59 (13)	C24—C23—H23B	109.0
C15—C10—C2	119.43 (13)	C22—C23—H23B	109.0

C11—C10—C2	121.97 (13)	H23A—C23—H23B	107.8
C10—C11—C12	120.06 (14)	C25—C24—C23	112.34 (12)
C10—C11—H11	120.0	C25—C24—H24A	109.1
C12—C11—H11	120.0	C23—C24—H24A	109.1
C13—C12—C11	120.69 (15)	C25—C24—H24B	109.1
C13—C12—H12	119.7	C23—C24—H24B	109.1
C11—C12—H12	119.7	H24A—C24—H24B	107.9
C14—C13—C12	119.50 (14)	C26—C25—C24	113.26 (14)
C14—C13—H13	120.2	C26—C25—H25A	108.9
C12—C13—H13	120.2	C24—C25—H25A	108.9
C13—C14—C15	120.24 (15)	C26—C25—H25B	108.9
C13—C14—H14	119.9	C24—C25—H25B	108.9
C15—C14—H14	119.9	H25A—C25—H25B	107.7
C14—C15—C10	120.91 (15)	C25—C26—H26A	109.5
C14—C15—H15	119.5	C25—C26—H26B	109.5
C10—C15—H15	119.5	H26A—C26—H26B	109.5
C17—C16—C21	117.68 (13)	C25—C26—H26C	109.5
C17—C16—C3	124.27 (12)	H26A—C26—H26C	109.5
C21—C16—C3	118.03 (13)	H26B—C26—H26C	109.5

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C15—H15...O119 <sup>i</sup>	0.95	2.61	3.4393 (19)	146

Symmetry code: (i)  $-x+2, -y+2, -z+2$ .