

2-(2,5-Dimethoxyphenyl)-4,5-diphenyl-1-(prop-2-en-1-yl)-1*H*-imidazole

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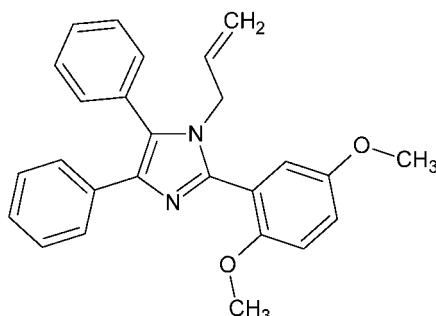
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(C-C) = 0.003$ Å; R factor = 0.047; wR factor = 0.125; data-to-parameter ratio = 15.4.

In the title compound, $C_{26}H_{24}N_2O_2$, the two phenyl and the 2,5-dimethoxyphenyl rings are inclined to the imidazole ring at dihedral angles of 30.38 (8), 56.59 (9) and 73.11 (9)°, respectively. In the crystal, molecules are linked by pairs of C—H···O interactions into centrosymmetric dimers with graph-set notation $R_2^2(8)$. C—H···π interactions are also observed.

Related literature

For chemical properties and applications of imidazoles with an unsaturated side chain, see, for example: Koszykowska *et al.* (2009); Berezin *et al.* (2009); Rambo *et al.* (2010); Min *et al.* (2006). For similar structures, see: Akkurt *et al.* (2013a,b); Mohamed *et al.* (2013a,b). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

| | |
|-------------------------|-----------------------------------|
| $C_{26}H_{24}N_2O_2$ | $\gamma = 107.772$ (2)° |
| $M_r = 396.47$ | $V = 1020.1$ (3) Å ³ |
| Triclinic, $P\bar{1}$ | $Z = 2$ |
| $a = 8.3117$ (14) Å | Mo $K\alpha$ radiation |
| $b = 10.5217$ (17) Å | $\mu = 0.08$ mm ⁻¹ |
| $c = 13.425$ (2) Å | $T = 100$ K |
| $\alpha = 105.938$ (2)° | $0.26 \times 0.16 \times 0.08$ mm |
| $\beta = 101.846$ (2)° | |

Data collection

| | |
|--|--|
| Bruker SMART APEX CCD area-detector diffractometer | 11527 measured reflections |
| Absorption correction: multi-scan (<i>SADABS</i> ; Sheldrick, 2004) | 4193 independent reflections |
| $T_{\min} = 0.979$, $T_{\max} = 0.993$ | 3184 reflections with $I > 2\sigma(I)$ |
| | $R_{\text{int}} = 0.036$ |

Refinement

| | |
|---------------------------------|---|
| $R[F^2 > 2\sigma(F^2)] = 0.047$ | 273 parameters |
| $wR(F^2) = 0.125$ | H-atom parameters constrained |
| $S = 1.05$ | $\Delta\rho_{\max} = 0.23$ e Å ⁻³ |
| 4193 reflections | $\Delta\rho_{\min} = -0.26$ e Å ⁻³ |

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

$Cg1$, $Cg2$ and $Cg4$ are the centroids of the N1/N2/C1–C3, C4–C9 and C19–C24 rings, respectively.

| $D-H \cdots A$ | $D-H$ | $H \cdots A$ | $D \cdots A$ | $D-H \cdots A$ |
|--------------------------|-------|--------------|--------------|----------------|
| $C20-H20 \cdots O1i$ | 0.95 | 2.54 | 3.354 (2) | 143 |
| $C14-H14 \cdots Cg2ii$ | 0.95 | 2.63 | 3.4083 (19) | 139 |
| $C25-H25B \cdots Cg1iii$ | 0.98 | 2.84 | 3.6337 (19) | 139 |
| $C26-H26C \cdots Cg4iv$ | 0.98 | 2.95 | 3.908 (2) | 166 |

Symmetry codes: (i) $-x, -y + 1, -z$; (ii) $-x, -y, -z + 1$; (iii) $-x + 1, -y + 1, -z + 1$; (iv) $-x + 1, -y + 1, -z$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; 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: *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2444).

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supporting information

Acta Cryst. (2013). E69, o1098–o1099 [https://doi.org/10.1107/S1600536813015936]

2-(2,5-Dimethoxyphenyl)-4,5-diphenyl-1-(prop-2-en-1-yl)-1*H*-imidazole

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S1. Comment

Recently, much attention has been devoted to vinyl and allyl N-substituted imidazole compounds due to their interesting properties and high reactivities. Such compounds in addition to their fluorescent properties (Berezin *et al.*, 2009; Rambo *et al.*, 2010) they can polymerize to obtain chromophoric polymers (Koszykowska *et al.*, 2009). In addition their quaternary salts are acting as ionic catalysts (Min *et al.*, 2006) which are widely used in green chemistry applications. In this context the title compound has been synthesized among series of allyl imidazole derivatives and herein we report its crystal structure.

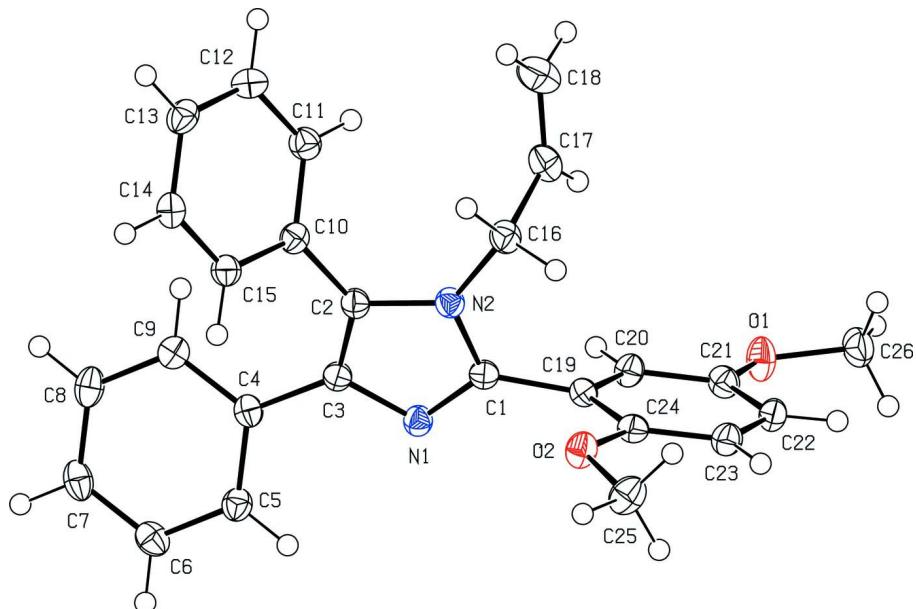
In the title compound (**I**, Fig. 1), the two phenyl (C4–C9 and C10–C15) and 2-(2,5-dimethoxyphenyl) (C19–C24) rings are inclined to the N1/N2/C1–C3 imidazole ring at angles of 30.38 (8), 56.59 (9) and 73.11 (9)°, respectively. All bond lengths and angles are normal and are corresponding to those reported in a similar structure (Akkurt *et al.*, 2013*a,b*; Mohamed *et al.*, 2013*a,b*). In the crystal the molecules are linked by C—H···O interactions into centrosymmetric dimers with graph-set notation R₂²(8) (Bernstein *et al.*, 1995). C—H···π interactions are also observed, Table 1, Fig2.

S2. Experimental

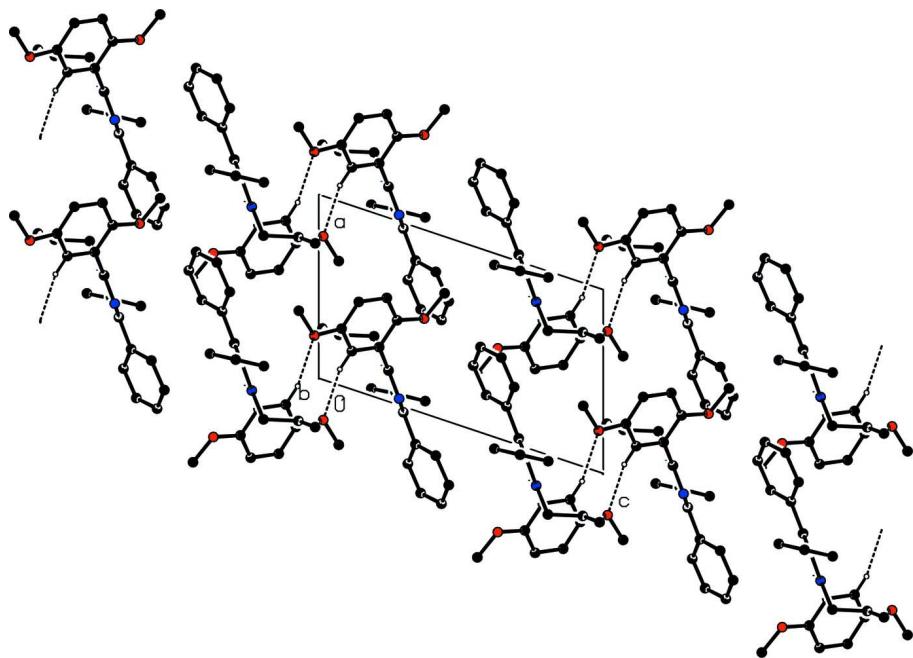
The title compound was synthesized according to our reported method (Mohamed *et al.* 2013*a*) in 85% yield. Colourless prisms suitable for X-ray analyses were obtained by slow evaporation of a solution of (**I**) in ethanol, m.p. 471–473 K.

S3. Refinement

All H atoms were placed in geometrically, with C—H = 0.95–0.99 Å, and refined as riding with $U_{\text{iso}}(\text{H})$ = 1.2 or $1.5U_{\text{eq}}(\text{C})$.

**Figure 1**

The molecular structure of the title compound with the atom numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

**Figure 2**

The hydrogen bonding and packing of the title compound viewing along the *b* axis. H atoms not involved in hydrogen bonds have been omitted for clarity.

2-(2,5-Dimethoxyphenyl)-4,5-diphenyl-1-(prop-2-en-1-yl)-1*H*-imidazole*Crystal data*

$C_{26}H_{24}N_2O_2$
 $M_r = 396.47$
Triclinic, $P\bar{1}$
Hall symbol: -P 1
 $a = 8.3117$ (14) Å
 $b = 10.5217$ (17) Å
 $c = 13.425$ (2) Å
 $\alpha = 105.938$ (2)°
 $\beta = 101.846$ (2)°
 $\gamma = 107.772$ (2)°
 $V = 1020.1$ (3) Å³

$Z = 2$
 $F(000) = 420$
 $D_x = 1.291$ Mg m⁻³
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2470 reflections
 $\theta = 2.2\text{--}26.3$ °
 $\mu = 0.08$ mm⁻¹
 $T = 100$ K
Prism, colourless
0.26 × 0.16 × 0.08 mm

Data collection

Bruker SMART APEX CCD area-detector
diffractometer
Radiation source: sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan
(SADABS; Sheldrick, 2004)
 $T_{\min} = 0.979$, $T_{\max} = 0.993$

11527 measured reflections
4193 independent reflections
3184 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.036$
 $\theta_{\max} = 26.5$ °, $\theta_{\min} = 1.7$ °
 $h = -10 \rightarrow 10$
 $k = -13 \rightarrow 13$
 $l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.047$
 $wR(F^2) = 0.125$
 $S = 1.05$
4193 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
 $w = 1/[\sigma^2(F_o^2) + (0.0613P)^2 + 0.1427P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.23$ e Å⁻³
 $\Delta\rho_{\min} = -0.26$ 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 e.s.d.'s 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 $F^2 > \sigma(F^2)$ 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 | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|----|--------------|--------------|--------------|----------------------------------|
| O1 | 0.22127 (15) | 0.57663 (13) | -0.01565 (9) | 0.0294 (4) |
| O2 | 0.51365 (14) | 0.51988 (12) | 0.37054 (9) | 0.0246 (3) |
| N1 | 0.03320 (16) | 0.34760 (14) | 0.28257 (10) | 0.0200 (4) |

| | | | | |
|------|--------------|---------------|---------------|------------|
| N2 | 0.19265 (16) | 0.21885 (14) | 0.23560 (10) | 0.0197 (4) |
| C1 | 0.1675 (2) | 0.34409 (16) | 0.24524 (12) | 0.0187 (4) |
| C2 | 0.0647 (2) | 0.13719 (17) | 0.26932 (12) | 0.0191 (5) |
| C3 | -0.0325 (2) | 0.21832 (16) | 0.29722 (12) | 0.0187 (5) |
| C4 | -0.1839 (2) | 0.18601 (17) | 0.34015 (12) | 0.0196 (5) |
| C5 | -0.2095 (2) | 0.29766 (17) | 0.41145 (13) | 0.0221 (5) |
| C6 | -0.3463 (2) | 0.26861 (19) | 0.45693 (13) | 0.0244 (5) |
| C7 | -0.4602 (2) | 0.12872 (19) | 0.43134 (14) | 0.0257 (5) |
| C8 | -0.4395 (2) | 0.01733 (19) | 0.35825 (14) | 0.0253 (5) |
| C9 | -0.3029 (2) | 0.04563 (17) | 0.31312 (13) | 0.0219 (5) |
| C10 | 0.05668 (19) | -0.00280 (17) | 0.27544 (13) | 0.0194 (4) |
| C11 | 0.0409 (2) | -0.11491 (17) | 0.18480 (13) | 0.0234 (5) |
| C12 | 0.0405 (2) | -0.24371 (18) | 0.19320 (14) | 0.0264 (5) |
| C13 | 0.0564 (2) | -0.26260 (18) | 0.29232 (14) | 0.0248 (5) |
| C14 | 0.0700 (2) | -0.15270 (17) | 0.38256 (13) | 0.0228 (5) |
| C15 | 0.0696 (2) | -0.02425 (17) | 0.37420 (13) | 0.0210 (5) |
| C16 | 0.3286 (2) | 0.18032 (18) | 0.19444 (13) | 0.0229 (5) |
| C17 | 0.2732 (2) | 0.12340 (19) | 0.07169 (14) | 0.0280 (5) |
| C18 | 0.2775 (3) | 0.0033 (2) | 0.01278 (16) | 0.0392 (7) |
| C19 | 0.2772 (2) | 0.45508 (16) | 0.21242 (13) | 0.0199 (5) |
| C20 | 0.2057 (2) | 0.47090 (17) | 0.11627 (13) | 0.0221 (5) |
| C21 | 0.3087 (2) | 0.56926 (17) | 0.08016 (13) | 0.0220 (5) |
| C22 | 0.4852 (2) | 0.65115 (17) | 0.14076 (14) | 0.0238 (5) |
| C23 | 0.5580 (2) | 0.63844 (17) | 0.23932 (13) | 0.0233 (5) |
| C24 | 0.4555 (2) | 0.54150 (16) | 0.27547 (13) | 0.0202 (5) |
| C25 | 0.6880 (2) | 0.61529 (18) | 0.44233 (14) | 0.0292 (5) |
| C26 | 0.3278 (2) | 0.64720 (19) | -0.07022 (15) | 0.0303 (6) |
| H5 | -0.13280 | 0.39400 | 0.42890 | 0.0270* |
| H6 | -0.36170 | 0.34510 | 0.50580 | 0.0290* |
| H7 | -0.55200 | 0.10910 | 0.46370 | 0.0310* |
| H8 | -0.51920 | -0.07860 | 0.33910 | 0.0300* |
| H9 | -0.28980 | -0.03130 | 0.26320 | 0.0260* |
| H11 | 0.03020 | -0.10310 | 0.11640 | 0.0280* |
| H12 | 0.02920 | -0.31920 | 0.13060 | 0.0320* |
| H13 | 0.05790 | -0.35020 | 0.29830 | 0.0300* |
| H14 | 0.07970 | -0.16520 | 0.45070 | 0.0270* |
| H15 | 0.07820 | 0.05010 | 0.43670 | 0.0250* |
| H16A | 0.35140 | 0.10690 | 0.22150 | 0.0270* |
| H16B | 0.44100 | 0.26590 | 0.22340 | 0.0270* |
| H17 | 0.23240 | 0.17810 | 0.03450 | 0.0340* |
| H18A | 0.31760 | -0.05390 | 0.04740 | 0.0470* |
| H18B | 0.24060 | -0.02650 | -0.06460 | 0.0470* |
| H20 | 0.08470 | 0.41400 | 0.07420 | 0.0270* |
| H22 | 0.55700 | 0.71610 | 0.11540 | 0.0290* |
| H23 | 0.67860 | 0.69670 | 0.28170 | 0.0280* |
| H25A | 0.77680 | 0.59950 | 0.40780 | 0.0440* |
| H25B | 0.70890 | 0.59740 | 0.51080 | 0.0440* |
| H25C | 0.69790 | 0.71440 | 0.45760 | 0.0440* |

| | | | | |
|------|---------|---------|----------|---------|
| H26A | 0.39130 | 0.74890 | -0.02480 | 0.0450* |
| H26B | 0.25120 | 0.63740 | -0.14020 | 0.0450* |
| H26C | 0.41400 | 0.60380 | -0.08310 | 0.0450* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|-------------|-------------|------------|
| O1 | 0.0266 (6) | 0.0360 (7) | 0.0281 (7) | 0.0075 (5) | 0.0080 (5) | 0.0209 (6) |
| O2 | 0.0216 (6) | 0.0252 (6) | 0.0223 (6) | 0.0044 (5) | 0.0028 (5) | 0.0098 (5) |
| N1 | 0.0190 (7) | 0.0203 (7) | 0.0193 (7) | 0.0059 (6) | 0.0055 (6) | 0.0074 (6) |
| N2 | 0.0188 (7) | 0.0205 (7) | 0.0210 (7) | 0.0079 (6) | 0.0073 (6) | 0.0080 (6) |
| C1 | 0.0183 (7) | 0.0192 (8) | 0.0169 (8) | 0.0064 (6) | 0.0042 (6) | 0.0059 (7) |
| C2 | 0.0181 (8) | 0.0204 (8) | 0.0156 (8) | 0.0047 (7) | 0.0040 (6) | 0.0060 (7) |
| C3 | 0.0189 (8) | 0.0187 (8) | 0.0167 (8) | 0.0058 (6) | 0.0046 (6) | 0.0062 (6) |
| C4 | 0.0189 (8) | 0.0233 (9) | 0.0193 (8) | 0.0092 (7) | 0.0060 (6) | 0.0106 (7) |
| C5 | 0.0215 (8) | 0.0219 (9) | 0.0253 (9) | 0.0090 (7) | 0.0080 (7) | 0.0108 (7) |
| C6 | 0.0245 (8) | 0.0308 (9) | 0.0249 (9) | 0.0160 (8) | 0.0102 (7) | 0.0125 (8) |
| C7 | 0.0202 (8) | 0.0357 (10) | 0.0300 (9) | 0.0133 (8) | 0.0119 (7) | 0.0189 (8) |
| C8 | 0.0177 (8) | 0.0282 (9) | 0.0298 (9) | 0.0054 (7) | 0.0051 (7) | 0.0159 (8) |
| C9 | 0.0202 (8) | 0.0221 (9) | 0.0226 (9) | 0.0078 (7) | 0.0050 (7) | 0.0086 (7) |
| C10 | 0.0152 (7) | 0.0200 (8) | 0.0215 (8) | 0.0058 (6) | 0.0044 (6) | 0.0073 (7) |
| C11 | 0.0237 (8) | 0.0248 (9) | 0.0213 (9) | 0.0090 (7) | 0.0068 (7) | 0.0085 (7) |
| C12 | 0.0296 (9) | 0.0217 (9) | 0.0248 (9) | 0.0100 (7) | 0.0080 (7) | 0.0043 (7) |
| C13 | 0.0241 (8) | 0.0206 (9) | 0.0326 (10) | 0.0099 (7) | 0.0093 (7) | 0.0123 (8) |
| C14 | 0.0205 (8) | 0.0256 (9) | 0.0236 (9) | 0.0073 (7) | 0.0077 (7) | 0.0121 (7) |
| C15 | 0.0180 (8) | 0.0216 (9) | 0.0226 (8) | 0.0068 (7) | 0.0069 (7) | 0.0072 (7) |
| C16 | 0.0194 (8) | 0.0249 (9) | 0.0260 (9) | 0.0093 (7) | 0.0084 (7) | 0.0096 (7) |
| C17 | 0.0249 (9) | 0.0345 (10) | 0.0263 (9) | 0.0113 (8) | 0.0113 (7) | 0.0114 (8) |
| C18 | 0.0452 (12) | 0.0426 (12) | 0.0293 (10) | 0.0187 (10) | 0.0155 (9) | 0.0073 (9) |
| C19 | 0.0194 (8) | 0.0190 (8) | 0.0224 (8) | 0.0073 (7) | 0.0100 (7) | 0.0067 (7) |
| C20 | 0.0197 (8) | 0.0213 (8) | 0.0234 (9) | 0.0056 (7) | 0.0057 (7) | 0.0088 (7) |
| C21 | 0.0243 (8) | 0.0246 (9) | 0.0202 (8) | 0.0111 (7) | 0.0073 (7) | 0.0104 (7) |
| C22 | 0.0253 (8) | 0.0201 (8) | 0.0293 (9) | 0.0078 (7) | 0.0132 (7) | 0.0115 (7) |
| C23 | 0.0206 (8) | 0.0222 (9) | 0.0249 (9) | 0.0062 (7) | 0.0069 (7) | 0.0077 (7) |
| C24 | 0.0214 (8) | 0.0198 (8) | 0.0201 (8) | 0.0092 (7) | 0.0070 (7) | 0.0063 (7) |
| C25 | 0.0243 (9) | 0.0263 (9) | 0.0281 (9) | 0.0045 (8) | -0.0003 (7) | 0.0087 (8) |
| C26 | 0.0363 (10) | 0.0328 (10) | 0.0315 (10) | 0.0149 (8) | 0.0173 (8) | 0.0193 (8) |

Geometric parameters (\AA , $^\circ$)

| | | | |
|--------|-----------|---------|-----------|
| O1—C21 | 1.376 (2) | C20—C21 | 1.394 (3) |
| O1—C26 | 1.427 (2) | C21—C22 | 1.382 (2) |
| O2—C24 | 1.374 (2) | C22—C23 | 1.397 (2) |
| O2—C25 | 1.430 (2) | C23—C24 | 1.383 (2) |
| N1—C1 | 1.320 (2) | C5—H5 | 0.9500 |
| N1—C3 | 1.387 (2) | C6—H6 | 0.9500 |
| N2—C1 | 1.372 (2) | C7—H7 | 0.9500 |
| N2—C2 | 1.388 (2) | C8—H8 | 0.9500 |

| | | | |
|-------------|-------------|---------------|--------|
| N2—C16 | 1.470 (2) | C9—H9 | 0.9500 |
| C1—C19 | 1.479 (2) | C11—H11 | 0.9500 |
| C2—C3 | 1.375 (2) | C12—H12 | 0.9500 |
| C2—C10 | 1.480 (3) | C13—H13 | 0.9500 |
| C3—C4 | 1.475 (2) | C14—H14 | 0.9500 |
| C4—C5 | 1.400 (2) | C15—H15 | 0.9500 |
| C4—C9 | 1.399 (3) | C16—H16A | 0.9900 |
| C5—C6 | 1.391 (3) | C16—H16B | 0.9900 |
| C6—C7 | 1.385 (3) | C17—H17 | 0.9500 |
| C7—C8 | 1.388 (3) | C18—H18A | 0.9500 |
| C8—C9 | 1.386 (3) | C18—H18B | 0.9500 |
| C10—C11 | 1.393 (2) | C20—H20 | 0.9500 |
| C10—C15 | 1.393 (2) | C22—H22 | 0.9500 |
| C11—C12 | 1.390 (3) | C23—H23 | 0.9500 |
| C12—C13 | 1.385 (3) | C25—H25A | 0.9800 |
| C13—C14 | 1.383 (2) | C25—H25B | 0.9800 |
| C14—C15 | 1.388 (3) | C25—H25C | 0.9800 |
| C16—C17 | 1.505 (2) | C26—H26A | 0.9800 |
| C17—C18 | 1.309 (3) | C26—H26B | 0.9800 |
| C19—C20 | 1.382 (2) | C26—H26C | 0.9800 |
| C19—C24 | 1.407 (2) | | |
| | | | |
| C21—O1—C26 | 117.36 (14) | C5—C6—H6 | 120.00 |
| C24—O2—C25 | 116.87 (14) | C7—C6—H6 | 120.00 |
| C1—N1—C3 | 105.42 (14) | C6—C7—H7 | 120.00 |
| C1—N2—C2 | 107.22 (14) | C8—C7—H7 | 120.00 |
| C1—N2—C16 | 125.18 (15) | C7—C8—H8 | 120.00 |
| C2—N2—C16 | 127.58 (15) | C9—C8—H8 | 120.00 |
| N1—C1—N2 | 111.60 (15) | C4—C9—H9 | 120.00 |
| N1—C1—C19 | 126.41 (16) | C8—C9—H9 | 120.00 |
| N2—C1—C19 | 121.96 (15) | C10—C11—H11 | 120.00 |
| N2—C2—C3 | 105.17 (15) | C12—C11—H11 | 120.00 |
| N2—C2—C10 | 122.53 (15) | C11—C12—H12 | 120.00 |
| C3—C2—C10 | 132.23 (16) | C13—C12—H12 | 120.00 |
| N1—C3—C2 | 110.59 (15) | C12—C13—H13 | 120.00 |
| N1—C3—C4 | 120.32 (15) | C14—C13—H13 | 120.00 |
| C2—C3—C4 | 129.08 (16) | C13—C14—H14 | 120.00 |
| C3—C4—C5 | 119.76 (16) | C15—C14—H14 | 120.00 |
| C3—C4—C9 | 121.91 (15) | C10—C15—H15 | 120.00 |
| C5—C4—C9 | 118.32 (16) | C14—C15—H15 | 120.00 |
| C4—C5—C6 | 120.51 (17) | N2—C16—H16A | 109.00 |
| C5—C6—C7 | 120.36 (16) | N2—C16—H16B | 109.00 |
| C6—C7—C8 | 119.68 (17) | C17—C16—H16A | 109.00 |
| C7—C8—C9 | 120.17 (18) | C17—C16—H16B | 109.00 |
| C4—C9—C8 | 120.90 (16) | H16A—C16—H16B | 108.00 |
| C2—C10—C11 | 121.70 (15) | C16—C17—H17 | 118.00 |
| C2—C10—C15 | 120.15 (15) | C18—C17—H17 | 118.00 |
| C11—C10—C15 | 118.13 (16) | C17—C18—H18A | 120.00 |

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| C10—C11—C12 | 120.84 (16) | C17—C18—H18B | 120.00 |
| C11—C12—C13 | 120.37 (16) | H18A—C18—H18B | 120.00 |
| C12—C13—C14 | 119.31 (17) | C19—C20—H20 | 120.00 |
| C13—C14—C15 | 120.39 (16) | C21—C20—H20 | 120.00 |
| C10—C15—C14 | 120.96 (15) | C21—C22—H22 | 120.00 |
| N2—C16—C17 | 112.28 (14) | C23—C22—H22 | 120.00 |
| C16—C17—C18 | 124.22 (18) | C22—C23—H23 | 120.00 |
| C1—C19—C20 | 119.57 (15) | C24—C23—H23 | 120.00 |
| C1—C19—C24 | 121.05 (15) | O2—C25—H25A | 109.00 |
| C20—C19—C24 | 119.34 (16) | O2—C25—H25B | 109.00 |
| C19—C20—C21 | 120.92 (16) | O2—C25—H25C | 109.00 |
| O1—C21—C20 | 115.32 (15) | H25A—C25—H25B | 109.00 |
| O1—C21—C22 | 125.10 (16) | H25A—C25—H25C | 109.00 |
| C20—C21—C22 | 119.58 (16) | H25B—C25—H25C | 109.00 |
| C21—C22—C23 | 120.05 (16) | O1—C26—H26A | 109.00 |
| C22—C23—C24 | 120.34 (16) | O1—C26—H26B | 109.00 |
| O2—C24—C19 | 115.12 (15) | O1—C26—H26C | 109.00 |
| O2—C24—C23 | 125.15 (15) | H26A—C26—H26B | 109.00 |
| C19—C24—C23 | 119.74 (15) | H26A—C26—H26C | 109.00 |
| C4—C5—H5 | 120.00 | H26B—C26—H26C | 109.00 |
| C6—C5—H5 | 120.00 | | |
| | | | |
| C26—O1—C21—C22 | 15.8 (2) | C2—C3—C4—C5 | 148.45 (17) |
| C26—O1—C21—C20 | -164.74 (15) | N1—C3—C4—C5 | -29.8 (2) |
| C25—O2—C24—C19 | -173.84 (15) | C3—C4—C5—C6 | -176.81 (15) |
| C25—O2—C24—C23 | 6.6 (2) | C3—C4—C9—C8 | 177.09 (16) |
| C1—N1—C3—C2 | 0.58 (17) | C9—C4—C5—C6 | 2.2 (2) |
| C1—N1—C3—C4 | 179.16 (14) | C5—C4—C9—C8 | -1.9 (2) |
| C3—N1—C1—N2 | -0.36 (17) | C4—C5—C6—C7 | -0.7 (3) |
| C3—N1—C1—C19 | 177.32 (15) | C5—C6—C7—C8 | -1.3 (3) |
| C16—N2—C1—C19 | 0.9 (2) | C6—C7—C8—C9 | 1.6 (3) |
| C16—N2—C2—C10 | 4.5 (2) | C7—C8—C9—C4 | 0.0 (3) |
| C2—N2—C1—C19 | -177.79 (14) | C2—C10—C11—C12 | 177.49 (17) |
| C16—N2—C2—C3 | -178.34 (14) | C11—C10—C15—C14 | 1.2 (3) |
| C1—N2—C2—C10 | -176.80 (14) | C2—C10—C15—C14 | -177.22 (16) |
| C16—N2—C1—N1 | 178.73 (13) | C15—C10—C11—C12 | -0.9 (3) |
| C2—N2—C16—C17 | 97.69 (19) | C10—C11—C12—C13 | -0.2 (3) |
| C1—N2—C16—C17 | -80.8 (2) | C11—C12—C13—C14 | 1.0 (3) |
| C2—N2—C1—N1 | 0.00 (17) | C12—C13—C14—C15 | -0.7 (3) |
| C1—N2—C2—C3 | 0.34 (16) | C13—C14—C15—C10 | -0.4 (3) |
| N1—C1—C19—C20 | -72.9 (2) | N2—C16—C17—C18 | -129.1 (2) |
| N1—C1—C19—C24 | 109.5 (2) | C1—C19—C24—C23 | 176.09 (16) |
| N2—C1—C19—C20 | 104.59 (19) | C20—C19—C24—O2 | 178.86 (15) |
| N2—C1—C19—C24 | -73.1 (2) | C1—C19—C24—O2 | -3.5 (2) |
| N2—C2—C10—C15 | 121.30 (18) | C24—C19—C20—C21 | 1.2 (3) |
| C3—C2—C10—C11 | 126.7 (2) | C20—C19—C24—C23 | -1.6 (3) |
| C3—C2—C10—C15 | -55.0 (3) | C1—C19—C20—C21 | -176.52 (16) |
| N2—C2—C10—C11 | -57.0 (2) | C19—C20—C21—C22 | 0.6 (3) |

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|--------------|--------------|-----------------|--------------|
| N2—C2—C3—C4 | −178.98 (15) | C19—C20—C21—O1 | −178.89 (16) |
| N2—C2—C3—N1 | −0.57 (17) | C20—C21—C22—C23 | −2.0 (3) |
| C10—C2—C3—N1 | 176.17 (16) | O1—C21—C22—C23 | 177.44 (16) |
| C10—C2—C3—C4 | −2.3 (3) | C21—C22—C23—C24 | 1.6 (3) |
| C2—C3—C4—C9 | −30.5 (3) | C22—C23—C24—C19 | 0.2 (3) |
| N1—C3—C4—C9 | 151.19 (15) | C22—C23—C24—O2 | 179.71 (16) |

Hydrogen-bond geometry (Å, °)

Cg1, Cg2 and Cg4 are the centroids of the N1/N2/C1—C3, C4—C9 and C19—C24 rings, respectively.

| D—H···A | D—H | H···A | D···A | D—H···A |
|-------------------------------|------|-------|-------------|---------|
| C20—H20···O1 ⁱ | 0.95 | 2.54 | 3.354 (2) | 143 |
| C14—H14···Cg2 ⁱⁱ | 0.95 | 2.63 | 3.4083 (19) | 139 |
| C25—H25B···Cg1 ⁱⁱⁱ | 0.98 | 2.84 | 3.6337 (19) | 139 |
| C26—H26C···Cg4 ^{iv} | 0.98 | 2.95 | 3.908 (2) | 166 |

Symmetry codes: (i) $-x, -y+1, -z$; (ii) $-x, -y, -z+1$; (iii) $-x+1, -y+1, -z+1$; (iv) $-x+1, -y+1, -z$.