# organic compounds

# 2-(3,4-Dimethoxyphenyl)-1-pentyl-4,5-diphenyl-1H-imidazole

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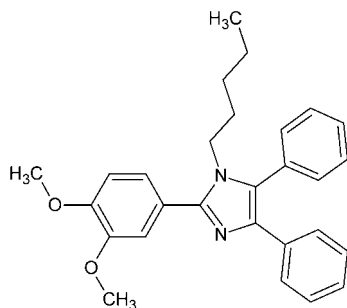Correspondence e-mail: shaabankamel@yahoo.com

The central imidazole ring in the title compound, $C_{28}H_{30}N_2O_2$, makes dihedral angles of 28.42 (13), 71.22 (15) and 29.50 (14)°, respectively, with the phenyl rings in the 4- and 5-positions and the 3,4-dimethoxyphenyl group. In the crystal, molecules are linked by C—H⋯O and C—H⋯N hydrogen bonds, weak $\pi$–$\pi$ stacking interactions [centroid–centroid distance = 3.760 (2) Å] and C—H⋯$\pi$ contacts, forming a three-dimensional network.

## Related literature

For medicinal and industrial applications of imidazole-containing compounds see: Oyeka & Gugnani (1992); Schrekker et al. (2013); Mital (2009); Juchau (1989); Rondu et al. (1997); Bousquet & Feldman (1999); Ueno et al. (1995); Jung & Huang (2000); Isobe et al. (2001). For similar structures, see: Akkurt et al. (2013); Mohamed et al. (2013).



## Experimental

### Crystal data

| | |
|---|---|
| $C_{28}H_{30}N_2O_2$ | $\gamma$ = 108.170 (6)° |
| $M_r$ = 426.54 | $V$ = 1131.8 (5) Å$^3$ |
| Triclinic, $P\bar{1}$ | $Z$ = 2 |
| $a$ = 8.900 (2) Å | Mo $K\alpha$ radiation |
| $b$ = 11.915 (3) Å | $\mu$ = 0.08 mm$^{-1}$ |
| $c$ = 12.009 (3) Å | $T$ = 150 K |
| $\alpha$ = 106.757 (6)° | 0.24 × 0.21 × 0.11 mm |
| $\beta$ = 96.007 (5)° | |

### Data collection

| | |
|---|---|
| Bruker APEX2000 CCD area-detector diffractometer | 8350 measured reflections |
| Absorption correction: multi-scan (SADABS; Bruker, 2011) | 3953 independent reflections |
| | 2219 reflections with $I > 2\sigma(I)$ |
| $T_{min}$ = 0.668, $T_{max}$ = 0.981 | $R_{int}$ = 0.086 |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.058 | 292 parameters |
| $wR(F^2)$ = 0.127 | H-atom parameters constrained |
| $S$ = 0.87 | $\Delta\rho_{max}$ = 0.25 e Å$^{-3}$ |
| 3953 reflections | $\Delta\rho_{min}$ = −0.25 e Å$^{-3}$ |

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

$Cg1$ is the centroid of the N1/N2/C1–C3 imidazole ring.

| $D$—H⋯$A$ | $D$—H | H⋯$A$ | $D$⋯$A$ | $D$—H⋯$A$ |
|---|---|---|---|---|
| C23—H23⋯O1[i] | 0.95 | 2.53 | 3.168 (4) | 125 |
| C27—H27A⋯N2[ii] | 0.98 | 2.51 | 3.474 (3) | 168 |
| C27—H27A⋯$Cg1$[ii] | 0.98 | 2.77 | 3.608 (3) | 144 |

Symmetry codes: (i) $x - 1, y - 1, z - 1$; (ii) $-x + 2, -y + 2, -z + 2$.

Data collection: SMART (Bruker, 2011); cell refinement: SAINT (Bruker, 2011); 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).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5371).

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# organic compounds

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# supplementary materials

## 2-(3,4-Dimethoxyphenyl)-1-pentyl-4,5-diphenyl-1*H*-imidazole

**Shaaban K. Mohamed, Mehmet Akkurt, Adel A. Marzouk, Kuldip Singh and Mustafa R. Albayati**

### 1. Comment

Many drugs contain an imidazole ring. Examples include butoconazole, clomidazole, clotrimazole, croconazole, econazole, fenticonazole, ketoconazole, isoconazole miconazole, neticonazole, omoconazole, oxiconazole, sertaconazole, sulconazole and tioconazole all of which act as antifungal drugs (Oyeka & Gugnani, 1992, Schrekker *et al.*, 2013). Antibiotic drugs such as metronidazole, tinidazole and nimorazole also contain imidazoles (Mital, 2009; Juchau, 1989). Moreover, 2-substituted imidazolines are used as synthetic intermediates (Rondu *et al.*, 1997), catalysts (Bousquet & Feldman, 1999), chiral auxiliaries (Ueno *et al.*, 1995), chiral catalysts (Jung & Huang, 2000) and ligands for asymmetric catalysis (Isobe *et al.*, 2001)in various synthetic reactions. Based on such facts, and as an extension of our work concerning the production bio-active heterocyclic compounds, we report in this study the synthesis and crystal structure of another imidazole derivative.

In the non-planar title compound (I), (Fig. 1), the dihedral angles between the (N1/N2/C1–C3) imidazole ring, and the two phenyl rings (C15–C20 and C21–C26) and the 3,4-dimethoxyphenyl group (C4–C9) are 28.42 (13), 71.22 (15) and 29.50 (14)°, respectively.

The N1–C10–C11–C12 and C11–C12–C13–C14 torsion angles are 173.6 (2) and 66.4 (4)°, respectively. The bond lengths and bond angles in (I) are normal and comparable to those reported for the similar compounds (Akkurt *et al.*, 2013; Mohamed *et al.*, 2013).

The crystal structure is stabilized by the intermolecular C—H⋯O, C—H⋯N hydrogen bonds (Table 1, Fig. 2), weak $\pi$-$\pi$ stacking interactions [$Cg2$⋯$Cg2$ (2 - *x*, 2 - *y*, 2 - *z*) = 3.760 (2) Å] between the benzene rings of adjacent 3,4-dimethoxy-phenyl groups and C—H⋯$\pi$ contacts (Table 1).

### 2. Experimental

The title compound was prepared by our previously reported method (Mohamed *et al.*, 2013). Single crystals sutiable for X-ray diffraction were grown up by the slow evaporation method from an ethanolic solution of (I). *M*.p. 424 K and 83% yield.

### 3. Refinement

H atoms were included in calculated positions and refined using a riding model with C—H = 0.95 - 0.99 Å and $U_{iso}$(H) = 1.5$U_{eq}$($C_{methyl}$) and = 1.2$U_{eq}$(C) for other H atoms. One reflection (0 0 1) was affected by the beam stop and was omitted from the refinement.

### Computing details

Data collection: *SMART* (Bruker, 2011); cell refinement: *SAINT* (Bruker, 2011); data reduction: *SAINT* (Bruker, 2011); 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).
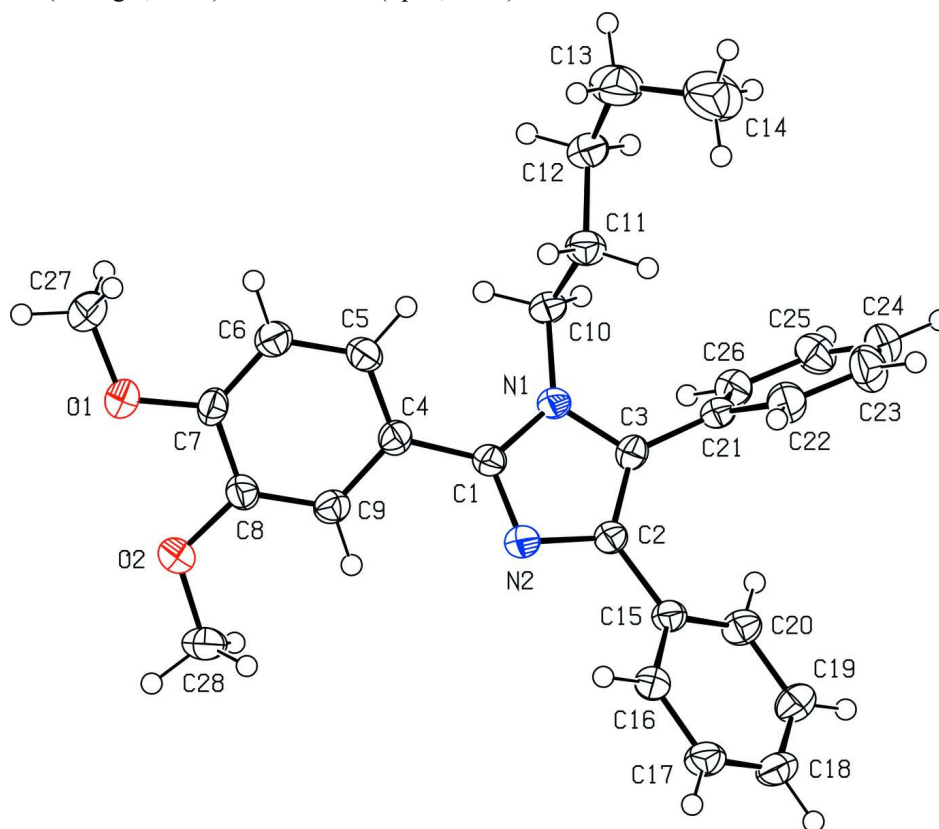


**Figure 1**

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.
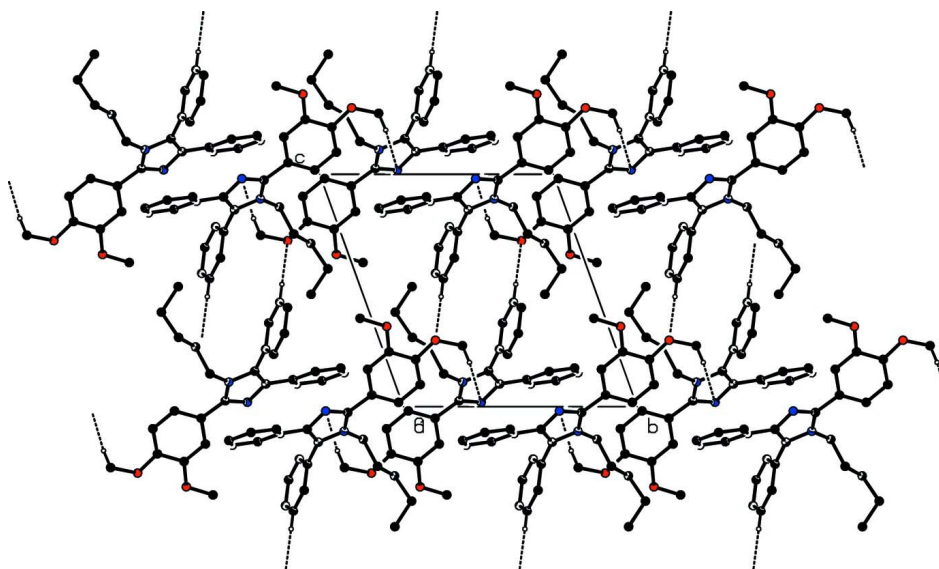


**Figure 2**

Crystal packing of the title compound viewed along the *a* axis. Hydrogen bonds are drawn as dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity.

**2-(3,4-Dimethoxyphenyl)-1-pentyl-4,5-diphenyl-1*H*-imidazole**

*Crystal data*

| | |
|---|---|
| $C_{28}H_{30}N_2O_2$ | $Z = 2$ |
| $M_r = 426.54$ | $F(000) = 456$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.252$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 8.900$ (2) Å | Cell parameters from 856 reflections |
| $b = 11.915$ (3) Å | $\theta = 2.5$–20.8° |
| $c = 12.009$ (3) Å | $\mu = 0.08$ mm$^{-1}$ |
| $\alpha = 106.757$ (6)° | $T = 150$ K |
| $\beta = 96.007$ (5)° | Block, colourless |
| $\gamma = 108.170$ (6)° | $0.24 \times 0.21 \times 0.11$ mm |
| $V = 1131.8$ (5) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Bruker APEX2000 CCD area-detector diffractometer | 8350 measured reflections |
| Radiation source: fine-focus sealed tube | 3953 independent reflections |
| Graphite monochromator | 2219 reflections with $I > 2\sigma(I)$ |
| $\varphi$ and $\omega$ scans | $R_{int} = 0.086$ |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2011) | $\theta_{max} = 25.0°$, $\theta_{min} = 1.9°$ |
| $T_{min} = 0.668$, $T_{max} = 0.981$ | $h = -10 \rightarrow 10$ |
| | $k = -13 \rightarrow 14$ |
| | $l = -14 \rightarrow 14$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | |
| $R[F^2 > 2\sigma(F^2)] = 0.058$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.127$ | |
| $S = 0.87$ | H-atom parameters constrained |
| 3953 reflections | $w = 1/[\sigma^2(F_o^2) + (0.0391P)^2]$ |
| 292 parameters | where $P = (F_o^2 + 2F_c^2)/3$ |
| 0 restraints | $(\Delta/\sigma)_{max} < 0.001$ |
| Primary atom site location: structure-invariant direct methods | $\Delta\rho_{max} = 0.25$ e Å$^{-3}$ |
| | $\Delta\rho_{min} = -0.25$ 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 (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 1.0678 (2) | 1.23924 (16) | 1.28583 (16) | 0.0391 (7) |
| O2 | 1.0748 (2) | 1.05208 (17) | 1.34508 (16) | 0.0404 (7) |
| N1 | 0.5735 (2) | 0.70894 (19) | 0.89430 (18) | 0.0259 (8) |
| N2 | 0.7629 (2) | 0.66063 (19) | 0.98101 (18) | 0.0278 (8) |

| | | | |
|---|---|---|---|
| C1 | 0.7160 (3) | 0.7530 (2) | 0.9748 (2) | 0.0262 (9) |
| C2 | 0.6472 (3) | 0.5534 (2) | 0.9023 (2) | 0.0257 (9) |
| C3 | 0.5296 (3) | 0.5811 (2) | 0.8472 (2) | 0.0272 (9) |
| C4 | 0.8031 (3) | 0.8829 (2) | 1.0501 (2) | 0.0268 (9) |
| C5 | 0.8063 (3) | 0.9857 (2) | 1.0185 (2) | 0.0305 (9) |
| C6 | 0.8932 (3) | 1.1059 (2) | 1.0950 (2) | 0.0316 (10) |
| C7 | 0.9794 (3) | 1.1250 (2) | 1.2033 (2) | 0.0287 (9) |
| C8 | 0.9822 (3) | 1.0229 (2) | 1.2361 (2) | 0.0291 (9) |
| C9 | 0.8945 (3) | 0.9045 (2) | 1.1609 (2) | 0.0282 (9) |
| C10 | 0.4779 (3) | 0.7773 (2) | 0.8591 (2) | 0.0302 (9) |
| C11 | 0.5026 (3) | 0.7972 (3) | 0.7431 (2) | 0.0338 (10) |
| C12 | 0.3887 (4) | 0.8550 (3) | 0.7021 (2) | 0.0409 (11) |
| C13 | 0.4153 (4) | 0.8893 (3) | 0.5935 (3) | 0.0567 (12) |
| C14 | 0.3796 (5) | 0.7783 (3) | 0.4835 (3) | 0.0731 (16) |
| C15 | 0.6611 (3) | 0.4312 (2) | 0.8838 (2) | 0.0269 (9) |
| C16 | 0.8124 (3) | 0.4217 (2) | 0.9029 (2) | 0.0306 (9) |
| C17 | 0.8291 (3) | 0.3083 (3) | 0.8889 (2) | 0.0348 (10) |
| C18 | 0.6946 (4) | 0.2014 (3) | 0.8543 (2) | 0.0355 (10) |
| C19 | 0.5440 (3) | 0.2083 (3) | 0.8336 (2) | 0.0360 (10) |
| C20 | 0.5276 (3) | 0.3225 (2) | 0.8490 (2) | 0.0316 (10) |
| C21 | 0.3856 (3) | 0.5008 (2) | 0.7528 (2) | 0.0285 (9) |
| C22 | 0.4042 (3) | 0.4467 (3) | 0.6400 (2) | 0.0371 (10) |
| C23 | 0.2726 (4) | 0.3681 (3) | 0.5509 (3) | 0.0432 (11) |
| C24 | 0.1200 (4) | 0.3430 (3) | 0.5736 (3) | 0.0392 (11) |
| C25 | 0.0999 (3) | 0.3960 (3) | 0.6849 (2) | 0.0370 (10) |
| C26 | 0.2314 (3) | 0.4741 (2) | 0.7744 (2) | 0.0330 (10) |
| C27 | 1.0564 (3) | 1.3462 (2) | 1.2624 (2) | 0.0410 (11) |
| C28 | 1.0836 (4) | 0.9506 (3) | 1.3800 (2) | 0.0448 (11) |
| H5 | 0.74750 | 0.97340 | 0.94260 | 0.0370* |
| H6 | 0.89280 | 1.17570 | 1.07190 | 0.0380* |
| H9 | 0.89540 | 0.83510 | 1.18430 | 0.0340* |
| H10A | 0.50770 | 0.86000 | 0.92220 | 0.0360* |
| H10B | 0.36180 | 0.73020 | 0.85150 | 0.0360* |
| H11A | 0.48440 | 0.71550 | 0.68170 | 0.0410* |
| H11B | 0.61570 | 0.85280 | 0.75310 | 0.0410* |
| H12A | 0.27640 | 0.79520 | 0.68590 | 0.0490* |
| H12B | 0.39940 | 0.93160 | 0.76790 | 0.0490* |
| H13A | 0.52930 | 0.94520 | 0.60760 | 0.0680* |
| H13B | 0.34560 | 0.93680 | 0.58040 | 0.0680* |
| H14A | 0.45340 | 0.73410 | 0.49350 | 0.1100* |
| H14B | 0.39440 | 0.80680 | 0.41520 | 0.1100* |
| H14C | 0.26760 | 0.72140 | 0.46970 | 0.1100* |
| H16 | 0.90650 | 0.49540 | 0.92620 | 0.0370* |
| H17 | 0.93380 | 0.30400 | 0.90320 | 0.0420* |
| H18 | 0.70560 | 0.12260 | 0.84460 | 0.0430* |
| H19 | 0.45050 | 0.13390 | 0.80840 | 0.0430* |
| H20 | 0.42250 | 0.32630 | 0.83550 | 0.0380* |
| H22 | 0.50970 | 0.46410 | 0.62370 | 0.0450* |
| H23 | 0.28690 | 0.33090 | 0.47340 | 0.0520* |

| | | | | |
|---|---|---|---|---|
| H24 | 0.02840 | 0.28870 | 0.51160 | 0.0470* |
| H25 | −0.00590 | 0.37880 | 0.70060 | 0.0440* |
| H26 | 0.21640 | 0.51020 | 0.85200 | 0.0400* |
| H27A | 1.09610 | 1.35060 | 1.19010 | 0.0610* |
| H27B | 1.12200 | 1.42190 | 1.32970 | 0.0610* |
| H27C | 0.94320 | 1.34030 | 1.25110 | 0.0610* |
| H28A | 0.97510 | 0.89910 | 1.38300 | 0.0670* |
| H28B | 1.15480 | 0.98290 | 1.45900 | 0.0670* |
| H28C | 1.12690 | 0.89930 | 1.32240 | 0.0670* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0477 (13) | 0.0262 (12) | 0.0363 (12) | 0.0116 (10) | −0.0006 (10) | 0.0057 (10) |
| O2 | 0.0492 (13) | 0.0345 (12) | 0.0327 (12) | 0.0150 (10) | −0.0060 (10) | 0.0095 (10) |
| N1 | 0.0273 (13) | 0.0266 (13) | 0.0258 (13) | 0.0145 (11) | 0.0038 (10) | 0.0073 (10) |
| N2 | 0.0298 (13) | 0.0273 (13) | 0.0285 (13) | 0.0127 (11) | 0.0052 (11) | 0.0102 (11) |
| C1 | 0.0301 (16) | 0.0270 (16) | 0.0233 (15) | 0.0122 (13) | 0.0046 (13) | 0.0094 (13) |
| C2 | 0.0266 (15) | 0.0259 (15) | 0.0257 (15) | 0.0119 (13) | 0.0053 (12) | 0.0079 (13) |
| C3 | 0.0313 (16) | 0.0249 (16) | 0.0255 (15) | 0.0129 (13) | 0.0068 (13) | 0.0054 (13) |
| C4 | 0.0268 (15) | 0.0273 (16) | 0.0264 (16) | 0.0130 (13) | 0.0065 (12) | 0.0056 (13) |
| C5 | 0.0304 (16) | 0.0346 (17) | 0.0267 (16) | 0.0136 (14) | 0.0020 (13) | 0.0100 (14) |
| C6 | 0.0310 (16) | 0.0291 (17) | 0.0357 (17) | 0.0119 (14) | 0.0064 (14) | 0.0114 (14) |
| C7 | 0.0278 (16) | 0.0226 (16) | 0.0303 (16) | 0.0092 (13) | 0.0040 (13) | 0.0017 (13) |
| C8 | 0.0308 (16) | 0.0304 (17) | 0.0243 (15) | 0.0138 (14) | 0.0023 (13) | 0.0047 (13) |
| C9 | 0.0304 (16) | 0.0282 (16) | 0.0295 (16) | 0.0140 (13) | 0.0081 (13) | 0.0105 (13) |
| C10 | 0.0317 (16) | 0.0296 (16) | 0.0332 (16) | 0.0178 (13) | 0.0050 (13) | 0.0096 (13) |
| C11 | 0.0352 (17) | 0.0371 (17) | 0.0342 (17) | 0.0185 (14) | 0.0072 (14) | 0.0137 (14) |
| C12 | 0.053 (2) | 0.0359 (18) | 0.0388 (18) | 0.0242 (16) | 0.0055 (15) | 0.0127 (15) |
| C13 | 0.072 (2) | 0.062 (2) | 0.049 (2) | 0.032 (2) | 0.0108 (19) | 0.0298 (19) |
| C14 | 0.097 (3) | 0.094 (3) | 0.046 (2) | 0.054 (3) | 0.018 (2) | 0.027 (2) |
| C15 | 0.0303 (16) | 0.0279 (16) | 0.0258 (15) | 0.0145 (13) | 0.0057 (13) | 0.0096 (13) |
| C16 | 0.0292 (16) | 0.0297 (16) | 0.0320 (16) | 0.0125 (13) | 0.0016 (13) | 0.0088 (13) |
| C17 | 0.0357 (18) | 0.0369 (18) | 0.0384 (18) | 0.0208 (15) | 0.0080 (14) | 0.0141 (15) |
| C18 | 0.0472 (19) | 0.0318 (17) | 0.0375 (18) | 0.0230 (16) | 0.0131 (15) | 0.0154 (14) |
| C19 | 0.0410 (19) | 0.0280 (17) | 0.0423 (18) | 0.0120 (14) | 0.0129 (15) | 0.0159 (14) |
| C20 | 0.0297 (16) | 0.0314 (17) | 0.0378 (17) | 0.0139 (14) | 0.0096 (14) | 0.0137 (14) |
| C21 | 0.0329 (16) | 0.0265 (16) | 0.0291 (16) | 0.0163 (13) | 0.0038 (13) | 0.0086 (13) |
| C22 | 0.0347 (17) | 0.0388 (18) | 0.0362 (18) | 0.0152 (15) | 0.0061 (15) | 0.0086 (15) |
| C23 | 0.043 (2) | 0.049 (2) | 0.0300 (18) | 0.0180 (17) | 0.0035 (15) | 0.0021 (15) |
| C24 | 0.0372 (19) | 0.0351 (18) | 0.0375 (19) | 0.0095 (15) | −0.0021 (15) | 0.0083 (15) |
| C25 | 0.0298 (17) | 0.0424 (19) | 0.0365 (18) | 0.0100 (15) | 0.0039 (14) | 0.0143 (15) |
| C26 | 0.0339 (17) | 0.0326 (17) | 0.0321 (16) | 0.0131 (14) | 0.0059 (14) | 0.0094 (14) |
| C27 | 0.050 (2) | 0.0277 (17) | 0.0433 (19) | 0.0128 (15) | 0.0063 (16) | 0.0117 (15) |
| C28 | 0.060 (2) | 0.046 (2) | 0.0379 (18) | 0.0316 (18) | 0.0031 (16) | 0.0171 (16) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C7 | 1.358 (3) | C24—C25 | 1.361 (4) |
| O1—C27 | 1.413 (3) | C25—C26 | 1.368 (4) |

| | | | |
|---|---|---|---|
| O2—C8 | 1.359 (3) | C5—H5 | 0.9500 |
| O2—C28 | 1.410 (4) | C6—H6 | 0.9500 |
| N1—C1 | 1.362 (3) | C9—H9 | 0.9500 |
| N1—C3 | 1.371 (3) | C10—H10A | 0.9900 |
| N1—C10 | 1.457 (3) | C10—H10B | 0.9900 |
| N2—C1 | 1.311 (3) | C11—H11A | 0.9900 |
| N2—C2 | 1.366 (3) | C11—H11B | 0.9900 |
| C1—C4 | 1.453 (3) | C12—H12A | 0.9900 |
| C2—C3 | 1.356 (4) | C12—H12B | 0.9900 |
| C2—C15 | 1.455 (4) | C13—H13A | 0.9900 |
| C3—C21 | 1.466 (4) | C13—H13B | 0.9900 |
| C4—C5 | 1.376 (3) | C14—H14A | 0.9800 |
| C4—C9 | 1.394 (3) | C14—H14B | 0.9800 |
| C5—C6 | 1.377 (3) | C14—H14C | 0.9800 |
| C6—C7 | 1.358 (3) | C16—H16 | 0.9500 |
| C7—C8 | 1.389 (3) | C17—H17 | 0.9500 |
| C8—C9 | 1.359 (3) | C18—H18 | 0.9500 |
| C10—C11 | 1.506 (3) | C19—H19 | 0.9500 |
| C11—C12 | 1.507 (5) | C20—H20 | 0.9500 |
| C12—C13 | 1.495 (4) | C22—H22 | 0.9500 |
| C13—C14 | 1.496 (5) | C23—H23 | 0.9500 |
| C15—C16 | 1.387 (4) | C24—H24 | 0.9500 |
| C15—C20 | 1.374 (4) | C25—H25 | 0.9500 |
| C16—C17 | 1.370 (4) | C26—H26 | 0.9500 |
| C17—C18 | 1.367 (5) | C27—H27A | 0.9800 |
| C18—C19 | 1.370 (5) | C27—H27B | 0.9800 |
| C19—C20 | 1.375 (4) | C27—H27C | 0.9800 |
| C21—C22 | 1.374 (3) | C28—H28A | 0.9800 |
| C21—C26 | 1.379 (4) | C28—H28B | 0.9800 |
| C22—C23 | 1.367 (4) | C28—H28C | 0.9800 |
| C23—C24 | 1.371 (5) | | |
| | | | |
| C7—O1—C27 | 117.52 (19) | C11—C10—H10B | 109.00 |
| C8—O2—C28 | 116.8 (2) | H10A—C10—H10B | 108.00 |
| C1—N1—C3 | 107.2 (2) | C10—C11—H11A | 109.00 |
| C1—N1—C10 | 129.6 (2) | C10—C11—H11B | 109.00 |
| C3—N1—C10 | 123.3 (2) | C12—C11—H11A | 109.00 |
| C1—N2—C2 | 106.1 (2) | C12—C11—H11B | 109.00 |
| N1—C1—N2 | 110.8 (2) | H11A—C11—H11B | 108.00 |
| N1—C1—C4 | 126.0 (2) | C11—C12—H12A | 108.00 |
| N2—C1—C4 | 123.1 (2) | C11—C12—H12B | 108.00 |
| N2—C2—C3 | 110.3 (2) | C13—C12—H12A | 109.00 |
| N2—C2—C15 | 121.4 (2) | C13—C12—H12B | 109.00 |
| C3—C2—C15 | 128.3 (2) | H12A—C12—H12B | 108.00 |
| N1—C3—C2 | 105.7 (2) | C12—C13—H13A | 109.00 |
| N1—C3—C21 | 123.1 (2) | C12—C13—H13B | 109.00 |
| C2—C3—C21 | 131.1 (2) | C14—C13—H13A | 109.00 |
| C1—C4—C5 | 124.9 (2) | C14—C13—H13B | 109.00 |
| C1—C4—C9 | 117.4 (2) | H13A—C13—H13B | 108.00 |

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| C5—C4—C9 | 117.7 (2) | C13—C14—H14A | 109.00 |
| C4—C5—C6 | 121.1 (2) | C13—C14—H14B | 109.00 |
| C5—C6—C7 | 120.2 (2) | C13—C14—H14C | 110.00 |
| O1—C7—C6 | 125.0 (2) | H14A—C14—H14B | 109.00 |
| O1—C7—C8 | 115.1 (2) | H14A—C14—H14C | 109.00 |
| C6—C7—C8 | 119.9 (2) | H14B—C14—H14C | 109.00 |
| O2—C8—C7 | 115.3 (2) | C15—C16—H16 | 119.00 |
| O2—C8—C9 | 125.1 (2) | C17—C16—H16 | 119.00 |
| C7—C8—C9 | 119.7 (2) | C16—C17—H17 | 120.00 |
| C4—C9—C8 | 121.3 (2) | C18—C17—H17 | 120.00 |
| N1—C10—C11 | 112.6 (2) | C17—C18—H18 | 120.00 |
| C10—C11—C12 | 111.4 (2) | C19—C18—H18 | 120.00 |
| C11—C12—C13 | 115.0 (3) | C18—C19—H19 | 120.00 |
| C12—C13—C14 | 113.5 (3) | C20—C19—H19 | 120.00 |
| C2—C15—C16 | 120.2 (2) | C15—C20—H20 | 120.00 |
| C2—C15—C20 | 122.1 (2) | C19—C20—H20 | 120.00 |
| C16—C15—C20 | 117.8 (2) | C21—C22—H22 | 120.00 |
| C15—C16—C17 | 121.5 (2) | C23—C22—H22 | 120.00 |
| C16—C17—C18 | 119.8 (3) | C22—C23—H23 | 120.00 |
| C17—C18—C19 | 119.8 (3) | C24—C23—H23 | 120.00 |
| C18—C19—C20 | 120.3 (3) | C23—C24—H24 | 120.00 |
| C15—C20—C19 | 120.9 (3) | C25—C24—H24 | 120.00 |
| C3—C21—C22 | 119.3 (2) | C24—C25—H25 | 120.00 |
| C3—C21—C26 | 122.0 (2) | C26—C25—H25 | 120.00 |
| C22—C21—C26 | 118.6 (2) | C21—C26—H26 | 120.00 |
| C21—C22—C23 | 120.7 (3) | C25—C26—H26 | 120.00 |
| C22—C23—C24 | 120.0 (3) | O1—C27—H27A | 109.00 |
| C23—C24—C25 | 119.9 (3) | O1—C27—H27B | 109.00 |
| C24—C25—C26 | 120.3 (3) | O1—C27—H27C | 110.00 |
| C21—C26—C25 | 120.5 (2) | H27A—C27—H27B | 109.00 |
| C4—C5—H5 | 119.00 | H27A—C27—H27C | 109.00 |
| C6—C5—H5 | 120.00 | H27B—C27—H27C | 109.00 |
| C5—C6—H6 | 120.00 | O2—C28—H28A | 109.00 |
| C7—C6—H6 | 120.00 | O2—C28—H28B | 109.00 |
| C4—C9—H9 | 119.00 | O2—C28—H28C | 109.00 |
| C8—C9—H9 | 119.00 | H28A—C28—H28B | 109.00 |
| N1—C10—H10A | 109.00 | H28A—C28—H28C | 109.00 |
| N1—C10—H10B | 109.00 | H28B—C28—H28C | 110.00 |
| C11—C10—H10A | 109.00 | | |
| | | | |
| C27—O1—C7—C6 | 6.7 (4) | C2—C3—C21—C26 | 109.2 (3) |
| C27—O1—C7—C8 | −173.8 (2) | C1—C4—C5—C6 | −179.5 (3) |
| C28—O2—C8—C7 | −178.5 (3) | C9—C4—C5—C6 | −1.8 (4) |
| C28—O2—C8—C9 | 2.2 (4) | C1—C4—C9—C8 | 178.7 (3) |
| C3—N1—C1—N2 | −0.3 (3) | C5—C4—C9—C8 | 0.9 (4) |
| C3—N1—C1—C4 | −177.0 (2) | C4—C5—C6—C7 | 0.8 (4) |
| C10—N1—C1—N2 | 179.9 (2) | C5—C6—C7—O1 | −179.3 (3) |
| C10—N1—C1—C4 | 3.2 (4) | C5—C6—C7—C8 | 1.2 (4) |
| C1—N1—C3—C2 | 0.5 (3) | O1—C7—C8—O2 | −1.0 (3) |

| | | | |
|---|---|---|---|
| C1—N1—C3—C21 | −177.1 (2) | O1—C7—C8—C9 | 178.4 (2) |
| C10—N1—C3—C2 | −179.6 (2) | C6—C7—C8—O2 | 178.6 (2) |
| C10—N1—C3—C21 | 2.8 (4) | C6—C7—C8—C9 | −2.0 (4) |
| C1—N1—C10—C11 | 100.4 (3) | O2—C8—C9—C4 | −179.7 (3) |
| C3—N1—C10—C11 | −79.4 (3) | C7—C8—C9—C4 | 1.0 (4) |
| C2—N2—C1—N1 | −0.1 (3) | N1—C10—C11—C12 | 173.6 (2) |
| C2—N2—C1—C4 | 176.7 (2) | C10—C11—C12—C13 | 174.5 (3) |
| C1—N2—C2—C3 | 0.5 (3) | C11—C12—C13—C14 | 66.4 (4) |
| C1—N2—C2—C15 | 178.9 (2) | C2—C15—C16—C17 | 178.5 (2) |
| N1—C1—C4—C5 | −33.0 (4) | C20—C15—C16—C17 | −0.7 (3) |
| N1—C1—C4—C9 | 149.3 (3) | C2—C15—C20—C19 | −179.2 (2) |
| N2—C1—C4—C5 | 150.7 (3) | C16—C15—C20—C19 | −0.1 (3) |
| N2—C1—C4—C9 | −27.0 (4) | C15—C16—C17—C18 | 0.6 (4) |
| N2—C2—C3—N1 | −0.6 (3) | C16—C17—C18—C19 | 0.1 (4) |
| N2—C2—C3—C21 | 176.7 (2) | C17—C18—C19—C20 | −0.9 (4) |
| C15—C2—C3—N1 | −178.9 (2) | C18—C19—C20—C15 | 0.8 (4) |
| C15—C2—C3—C21 | −1.5 (5) | C3—C21—C22—C23 | 177.9 (3) |
| N2—C2—C15—C16 | −27.4 (3) | C26—C21—C22—C23 | 0.1 (5) |
| N2—C2—C15—C20 | 151.7 (2) | C3—C21—C26—C25 | −178.2 (3) |
| C3—C2—C15—C16 | 150.8 (3) | C22—C21—C26—C25 | −0.5 (4) |
| C3—C2—C15—C20 | −30.2 (4) | C21—C22—C23—C24 | 0.3 (5) |
| N1—C3—C21—C22 | 108.4 (3) | C22—C23—C24—C25 | −0.3 (5) |
| N1—C3—C21—C26 | −73.9 (3) | C23—C24—C25—C26 | −0.1 (5) |
| C2—C3—C21—C22 | −68.5 (4) | C24—C25—C26—C21 | 0.5 (5) |

*Hydrogen-bond geometry (Å, º)*

Cg1 is the centroid of the N1/N2/C1–C3 imidazole ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C23—H23···O1[i] | 0.95 | 2.53 | 3.168 (4) | 125 |
| C27—H27*A*···N2[ii] | 0.98 | 2.51 | 3.474 (3) | 168 |
| C27—H27*A*···Cg1[ii] | 0.98 | 2.77 | 3.608 (3) | 144 |

Symmetry codes: (i) *x*−1, *y*−1, *z*−1; (ii) −*x*+2, −*y*+2, −*z*+2.