

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

(2E)-3-(1,3-Diphenyl-1H-pyrazol-4-yl)-1-phenylprop-2-en-1-one

 Hoong-Kun Fun,^{a,*} Madhukar Hemamalini,^a Shridhar Malladi,^b Pradeep Poojari^b and Arun M Isloor^b
^aX-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, and ^bDepartment of Chemistry, National Institute of Technology, Karnataka, Surathkal, Mangalore 575 025, India

Correspondence e-mail: hkfun@usm.my

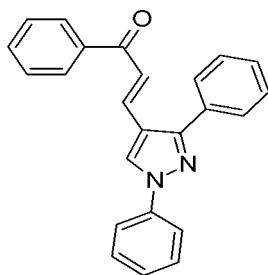
Received 14 June 2011; accepted 15 June 2011

 Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.001$ Å; R factor = 0.044; wR factor = 0.131; data-to-parameter ratio = 30.2.

In the title compound, $\text{C}_{24}\text{H}_{18}\text{N}_2\text{O}$, the pyrazole ring is essentially planar [maximum deviation = 0.004 (1) Å] and makes dihedral angles of 18.07 (4), 48.60 (4) and 9.13 (5)° with the phenyl rings. In the crystal, adjacent molecules are connected *via* intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds, forming dimers. Furthermore, the crystal structure is stabilized by weak $\text{C}-\text{H}\cdots\pi$ and $\pi-\pi$ interactions, with centroid-centroid distances of 3.6808 (5) Å.

Related literature

For applications of pyrazoles, see: Patel *et al.* (2004); Isloor *et al.* (2009); Vijesh *et al.* (2010); Sharma *et al.* (2010); Rostom *et al.* (2003); Ghorab *et al.* (2010); Amnekar & Bhusari (2010). For the synthetic procedure, see: Sharma *et al.* (2010). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986).



Experimental

Crystal data

$\text{C}_{24}\text{H}_{18}\text{N}_2\text{O}$	$a = 8.1027$ (2) Å
$M_r = 350.40$	$b = 9.3157$ (2) Å
Triclinic, $P\bar{1}$	$c = 12.9634$ (3) Å

* Thomson Reuters ResearcherID: A-3561-2009.

$\alpha = 73.630$ (1)°
$\beta = 74.713$ (1)°
$\gamma = 74.820$ (1)°
$V = 886.83$ (4) Å ³
$Z = 2$

Mo $K\alpha$ radiation
$\mu = 0.08$ mm ⁻¹
$T = 100$ K
$0.66 \times 0.23 \times 0.16$ mm

Data collection

Bruker SMART APEXII CCD	27273 measured reflections
area-detector diffractometer	7371 independent reflections
Absorption correction: multi-scan	6190 reflections with $I > 2\sigma(I)$
(SADABS; Bruker, 2009)	$R_{\text{int}} = 0.024$
$T_{\text{min}} = 0.949$, $T_{\text{max}} = 0.988$	

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$	244 parameters
$wR(F^2) = 0.131$	H-atom parameters constrained
$S = 1.04$	$\Delta\rho_{\text{max}} = 0.50$ e Å ⁻³
7371 reflections	$\Delta\rho_{\text{min}} = -0.30$ e Å ⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$\text{Cg}2$ and $\text{Cg}3$ are the centroids of the $\text{C}20-\text{C}25$ and $\text{C}13-\text{C}18$ rings, respectively.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C}12-\text{H}12A\cdots\text{O}1^i$	0.95	2.27	3.2019 (11)	167
$\text{C}15-\text{H}15A\cdots\text{Cg}2^{ii}$	0.95	2.81	3.6171 (9)	143
$\text{C}2-\text{H}2A\cdots\text{Cg}3^{iii}$	0.95	2.63	3.4304 (9)	143

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

HKF and MH thank the Malaysian Government and Universiti Sains Malaysia for the Research University Grant No. 1001/PFIZIK/811160. MH also thanks the Universiti Sains Malaysia for a post-doctoral research fellowship. AMI thanks the Department of Atomic Energy, Board for Research in Nuclear Sciences, Government of India, for a Young Scientist's award.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2615).

References

- Amnekar, N. D. & Bhusari, K. P. (2010). *Eur. J. Med. Chem.* **45**, 149–159.
- Bruker (2009). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Cosier, J. & Glazer, A. M. (1986). *J. Appl. Cryst.* **19**, 105–107.
- Ghorab, M. M., Ragab, F. A., Alqasoumi, S. I., Alafeefy, A. M. & Aboulmagd, S. A. (2010). *Eur. J. Med. Chem.* **45**, 171–178.
- Isloor, A. M., Kalluraya, B. & Shetty, P. (2009). *Eur. J. Med. Chem.* **44**, 3784–3787.
- Patel, M. V., Bell, R., Majest, S., Henry, R. & Kolasa, T. (2004). *J. Org. Chem.* **69**, 7058–7065.
- Rostom, S. A. F., Shalaby, M. A. & El-Demellawy, M. A. (2003). *Eur. J. Med. Chem.* **38**, 959–974.
- Sharma, P. K., Kumar, S., Kumar, P., Kaushik, P., Kaushik, D., Dhingra, Y. & Aneja, K. R. (2010). *Eur. J. Med. Chem.* **45**, 2650–2655.

Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.

Vijesh, A. M., Isloor, A. M., Prabhu, V., Ahmad, S. & Malladi, S. (2010). *Eur. J. Med. Chem.* **45**, 5460–5464.

supporting information

Acta Cryst. (2011). E67, o1745–o1746 [doi:10.1107/S1600536811023282]

(2E)-3-(1,3-Diphenyl-1H-pyrazol-4-yl)-1-phenylprop-2-en-1-one**Hoong-Kun Fun, Madhukar Hemamalini, Shridhar Malladi, Pradeep Poojari and Arun M Isloor****S1. Comment**

Pyrazoles are a novel class of heterocyclic compounds possessing wide variety of applications in the agrochemical and pharmaceutical industries (Patel *et al.*, 2004). Derivatives of pyrazoles are found to show good antibacterial (Isloor *et al.*, 2009; Vijesh *et al.*, 2010), anti-inflammatory (Sharma *et al.*, 2010), analgesic (Rostom *et al.*, 2003), anticancer, radioprotective (Ghorab *et al.*, 2010) and anti-convulsant activities (Amnekar *et al.*, 2010). Prompted by these diverse activities of pyrazole derivatives, we have synthesized the title compound to study its crystal structure.

In the title compound (Fig. 1), the pyrazole (N1/N2/C10–C12) group is essentially planar, with a maximum deviation of 0.004 (1) Å for atom C12, and makes dihedral angles of 18.07 (4)°, 48.60 (4)° and 9.13 (5)° with the adjacent C1–C6, C13–C18) and C19–C24 phenyl rings, respectively.

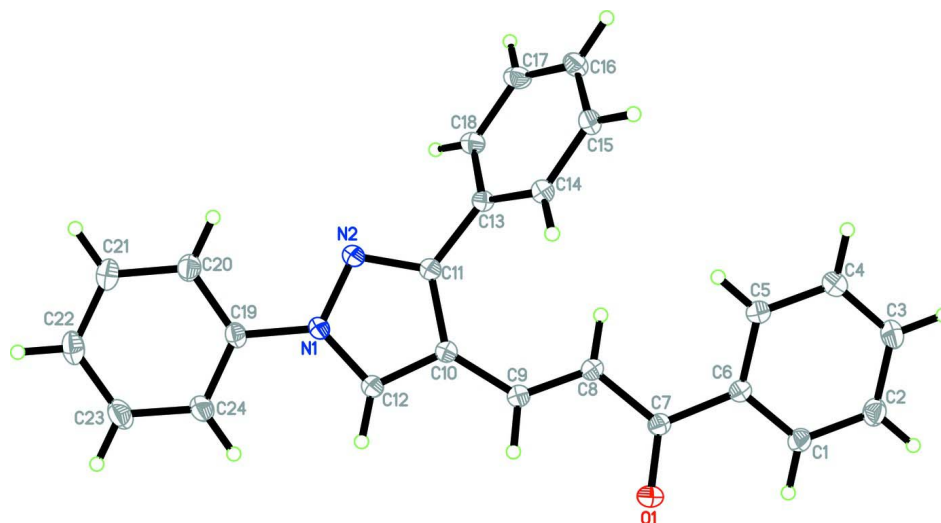
In the crystal structure (Fig. 2), adjacent molecules are connected *via* intermolecular C12—H12A···O1 (Table 1) hydrogen bonds forming dimers. Furthermore, the crystal structure is stabilized by weak π – π interactions between the pyrazole (N1/N2/C10–C12) and phenyl (C19–C24) rings [Cg···Cg = 3.6808 (5) Å; -x, 2-y, 1-z] and C—H··· π (Table 1) interactions, involving the centroids of the C20–C25 (Cg2) and C13–C18 (Cg3) rings.

S2. Experimental

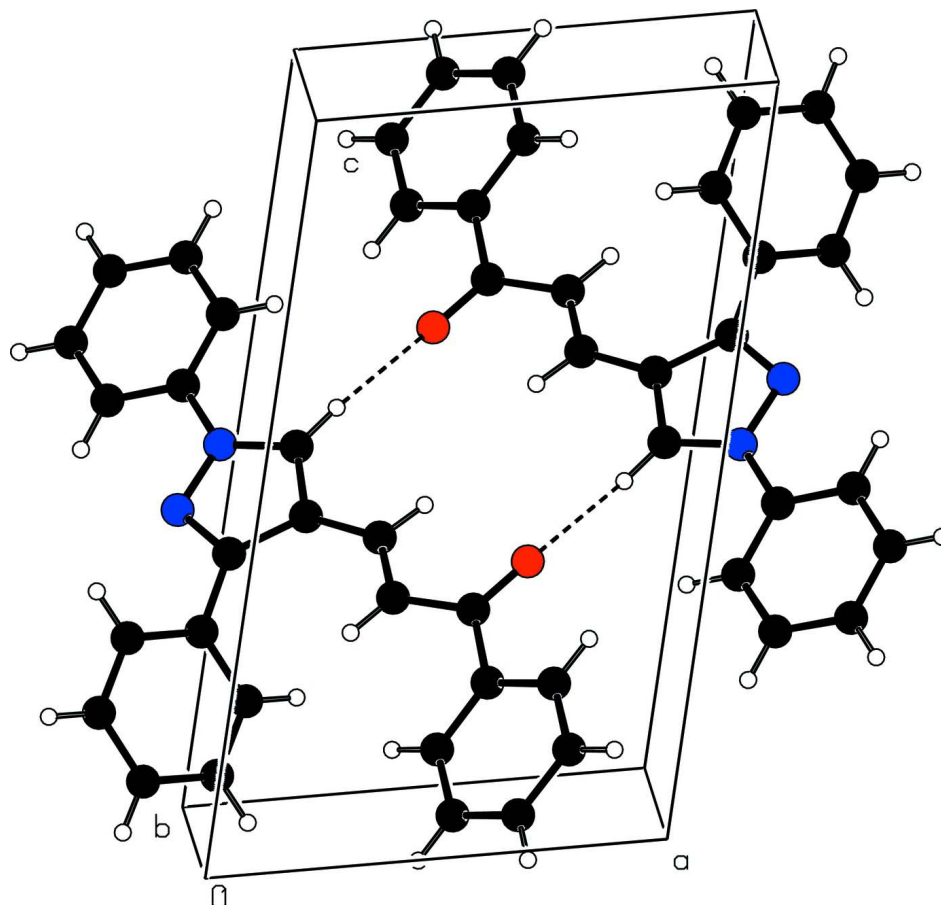
To a cold stirred mixture of methanol (20 ml) and sodium hydroxide (12.09 mmol) was added acetophenone (4.03 mmol). The reaction mixture was stirred for 10 min. To this solution was added formyl pyrazole (4.03 mmol) followed by tetrahydrofuran (30 ml). The solution was further stirred for 2 h at 0 °C and then at room temperature for 5 h. It was then poured into ice cold water. The resulting solution was neutralized with diluted HCl. The solid that separated out was filtered, washed with water, dried and crystallized from ethanol. Yield: 1.15 g, 81.5 %. M. p.: 406–408 K (Sharma *et al.*, 2010).

S3. Refinement

All hydrogen atoms were positioned geometrically [C–H = 0.95 Å] and were refined using a riding model, with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$.

**Figure 1**

The asymmetric unit of the title compound, showing 30% probability displacement ellipsoids.

**Figure 2**

The crystal packing of the title compound. Intermolecular hydrogen bonds are shown as dashed lines.

(2E)-3-(1,3-Diphenyl-1H-pyrazol-4-yl)-1-phenylprop-2-en-1-one*Crystal data*

$C_{24}H_{18}N_2O$	$Z = 2$
$M_r = 350.40$	$F(000) = 368$
Triclinic, $P\bar{1}$	$D_x = 1.312 \text{ Mg m}^{-3}$
Hall symbol: $-P\ 1$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 8.1027 (2) \text{ \AA}$	Cell parameters from 9964 reflections
$b = 9.3157 (2) \text{ \AA}$	$\theta = 2.3\text{--}34.3^\circ$
$c = 12.9634 (3) \text{ \AA}$	$\mu = 0.08 \text{ mm}^{-1}$
$\alpha = 73.630 (1)^\circ$	$T = 100 \text{ K}$
$\beta = 74.713 (1)^\circ$	Block, colourless
$\gamma = 74.820 (1)^\circ$	$0.66 \times 0.23 \times 0.16 \text{ mm}$
$V = 886.83 (4) \text{ \AA}^3$	

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	27273 measured reflections
Radiation source: fine-focus sealed tube	7371 independent reflections
Graphite monochromator	6190 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{\text{int}} = 0.024$
Absorption correction: multi-scan (<i>SADABS</i> ; Bruker, 2009)	$\theta_{\text{max}} = 34.4^\circ$, $\theta_{\text{min}} = 1.7^\circ$
$T_{\text{min}} = 0.949$, $T_{\text{max}} = 0.988$	$h = -12 \rightarrow 12$
	$k = -14 \rightarrow 14$
	$l = -20 \rightarrow 19$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.044$	H-atom parameters constrained
$wR(F^2) = 0.131$	$w = 1/[\sigma^2(F_o^2) + (0.0751P)^2 + 0.1576P]$
$S = 1.04$	where $P = (F_o^2 + 2F_c^2)/3$
7371 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
244 parameters	$\Delta\rho_{\text{max}} = 0.50 \text{ e \AA}^{-3}$
0 restraints	$\Delta\rho_{\text{min}} = -0.30 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.62674 (8)	0.29923 (7)	0.35790 (5)	0.02264 (13)
N1	-0.05079 (9)	0.77669 (8)	0.50245 (5)	0.01568 (12)

N2	-0.12324 (9)	0.77040 (8)	0.42026 (5)	0.01623 (12)
C1	0.70994 (10)	0.10968 (9)	0.21010 (6)	0.01851 (14)
H1A	0.7701	0.0780	0.2690	0.022*
C2	0.75836 (11)	0.02845 (9)	0.12812 (7)	0.02144 (15)
H2A	0.8514	-0.0584	0.1312	0.026*
C3	0.67086 (12)	0.07414 (10)	0.04162 (7)	0.02281 (16)
H3A	0.7029	0.0177	-0.0137	0.027*
C4	0.53661 (12)	0.20236 (11)	0.03622 (7)	0.02424 (16)
H4A	0.4781	0.2345	-0.0235	0.029*
C5	0.48746 (11)	0.28408 (10)	0.11820 (7)	0.02067 (15)
H5A	0.3953	0.3716	0.1142	0.025*
C6	0.57315 (10)	0.23783 (8)	0.20632 (6)	0.01585 (13)
C7	0.52409 (10)	0.31976 (8)	0.29762 (6)	0.01587 (13)
C8	0.35228 (10)	0.42396 (9)	0.31234 (6)	0.01641 (13)
H8A	0.2708	0.4290	0.2698	0.020*
C9	0.31000 (10)	0.51223 (9)	0.38577 (6)	0.01634 (13)
H9A	0.3974	0.5030	0.4251	0.020*
C10	0.14917 (10)	0.61871 (8)	0.41212 (6)	0.01493 (12)
C11	-0.00317 (10)	0.67559 (8)	0.36519 (6)	0.01476 (12)
C12	0.11129 (10)	0.68879 (8)	0.49939 (6)	0.01588 (13)
H12A	0.1858	0.6770	0.5481	0.019*
C13	-0.04028 (10)	0.65220 (8)	0.26639 (6)	0.01507 (12)
C14	0.08119 (10)	0.67017 (9)	0.16654 (6)	0.01730 (13)
H14A	0.1920	0.6890	0.1640	0.021*
C15	0.04095 (11)	0.66063 (9)	0.07101 (6)	0.02009 (14)
H15A	0.1240	0.6731	0.0037	0.024*
C16	-0.12143 (12)	0.63272 (10)	0.07439 (7)	0.02177 (15)
H16A	-0.1498	0.6271	0.0092	0.026*
C17	-0.24183 (11)	0.61317 (9)	0.17338 (7)	0.02090 (15)
H17A	-0.3518	0.5928	0.1758	0.025*
C18	-0.20240 (10)	0.62324 (9)	0.26905 (6)	0.01804 (14)
H18A	-0.2858	0.6104	0.3362	0.022*
C19	-0.14395 (10)	0.87250 (9)	0.57610 (6)	0.01661 (13)
C20	-0.29759 (11)	0.97422 (9)	0.55476 (7)	0.01987 (14)
H20A	-0.3394	0.9800	0.4915	0.024*
C21	-0.38932 (12)	1.06744 (10)	0.62720 (7)	0.02283 (16)
H21A	-0.4949	1.1362	0.6136	0.027*
C22	-0.32750 (12)	1.06055 (10)	0.71912 (8)	0.02431 (17)
H22A	-0.3906	1.1241	0.7684	0.029*
C23	-0.17285 (12)	0.96010 (12)	0.73845 (8)	0.02685 (18)
H23A	-0.1295	0.9565	0.8007	0.032*
C24	-0.08031 (11)	0.86448 (11)	0.66779 (7)	0.02333 (16)
H24A	0.0245	0.7949	0.6820	0.028*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0202 (3)	0.0266 (3)	0.0242 (3)	0.0010 (2)	-0.0109 (2)	-0.0099 (2)

N1	0.0156 (3)	0.0183 (3)	0.0144 (3)	-0.0022 (2)	-0.0034 (2)	-0.0065 (2)
N2	0.0160 (3)	0.0189 (3)	0.0151 (3)	-0.0022 (2)	-0.0045 (2)	-0.0059 (2)
C1	0.0177 (3)	0.0176 (3)	0.0184 (3)	0.0004 (2)	-0.0047 (2)	-0.0039 (2)
C2	0.0221 (4)	0.0182 (3)	0.0214 (3)	0.0009 (3)	-0.0033 (3)	-0.0062 (3)
C3	0.0245 (4)	0.0245 (4)	0.0203 (3)	-0.0032 (3)	-0.0022 (3)	-0.0103 (3)
C4	0.0233 (4)	0.0310 (4)	0.0191 (3)	-0.0001 (3)	-0.0069 (3)	-0.0093 (3)
C5	0.0184 (3)	0.0238 (4)	0.0193 (3)	0.0014 (3)	-0.0069 (3)	-0.0066 (3)
C6	0.0149 (3)	0.0161 (3)	0.0163 (3)	-0.0012 (2)	-0.0042 (2)	-0.0042 (2)
C7	0.0152 (3)	0.0157 (3)	0.0169 (3)	-0.0017 (2)	-0.0048 (2)	-0.0040 (2)
C8	0.0144 (3)	0.0171 (3)	0.0183 (3)	-0.0010 (2)	-0.0046 (2)	-0.0056 (2)
C9	0.0148 (3)	0.0180 (3)	0.0166 (3)	-0.0020 (2)	-0.0041 (2)	-0.0050 (2)
C10	0.0144 (3)	0.0158 (3)	0.0152 (3)	-0.0024 (2)	-0.0035 (2)	-0.0046 (2)
C11	0.0151 (3)	0.0156 (3)	0.0140 (3)	-0.0028 (2)	-0.0035 (2)	-0.0036 (2)
C12	0.0152 (3)	0.0180 (3)	0.0153 (3)	-0.0025 (2)	-0.0036 (2)	-0.0054 (2)
C13	0.0157 (3)	0.0149 (3)	0.0151 (3)	-0.0014 (2)	-0.0049 (2)	-0.0042 (2)
C14	0.0170 (3)	0.0189 (3)	0.0161 (3)	-0.0016 (2)	-0.0040 (2)	-0.0054 (2)
C15	0.0225 (3)	0.0214 (3)	0.0162 (3)	0.0002 (3)	-0.0047 (3)	-0.0076 (3)
C16	0.0265 (4)	0.0213 (3)	0.0207 (3)	-0.0010 (3)	-0.0099 (3)	-0.0087 (3)
C17	0.0226 (4)	0.0206 (3)	0.0231 (4)	-0.0050 (3)	-0.0104 (3)	-0.0048 (3)
C18	0.0180 (3)	0.0190 (3)	0.0182 (3)	-0.0039 (2)	-0.0060 (3)	-0.0037 (2)
C19	0.0165 (3)	0.0183 (3)	0.0160 (3)	-0.0045 (2)	-0.0007 (2)	-0.0070 (2)
C20	0.0200 (3)	0.0191 (3)	0.0196 (3)	-0.0020 (3)	-0.0025 (3)	-0.0065 (3)
C21	0.0220 (4)	0.0198 (3)	0.0249 (4)	-0.0023 (3)	0.0004 (3)	-0.0089 (3)
C22	0.0237 (4)	0.0251 (4)	0.0257 (4)	-0.0073 (3)	0.0036 (3)	-0.0140 (3)
C23	0.0239 (4)	0.0377 (5)	0.0240 (4)	-0.0064 (3)	-0.0012 (3)	-0.0182 (3)
C24	0.0198 (4)	0.0321 (4)	0.0212 (4)	-0.0022 (3)	-0.0038 (3)	-0.0143 (3)

Geometric parameters (Å, °)

O1—C7	1.2305 (9)	C11—C13	1.4742 (10)
N1—C12	1.3508 (10)	C12—H12A	0.9500
N1—N2	1.3661 (8)	C13—C18	1.3985 (11)
N1—C19	1.4232 (9)	C13—C14	1.4016 (11)
N2—C11	1.3325 (10)	C14—C15	1.3921 (10)
C1—C2	1.3906 (11)	C14—H14A	0.9500
C1—C6	1.3995 (11)	C15—C16	1.3939 (12)
C1—H1A	0.9500	C15—H15A	0.9500
C2—C3	1.3904 (12)	C16—C17	1.3903 (13)
C2—H2A	0.9500	C16—H16A	0.9500
C3—C4	1.3883 (13)	C17—C18	1.3926 (11)
C3—H3A	0.9500	C17—H17A	0.9500
C4—C5	1.3935 (11)	C18—H18A	0.9500
C4—H4A	0.9500	C19—C24	1.3918 (11)
C5—C6	1.3989 (11)	C19—C20	1.3930 (11)
C5—H5A	0.9500	C20—C21	1.3936 (11)
C6—C7	1.4978 (10)	C20—H20A	0.9500
C7—C8	1.4742 (11)	C21—C22	1.3892 (13)
C8—C9	1.3496 (10)	C21—H21A	0.9500

C8—H8A	0.9500	C22—C23	1.3885 (14)
C9—C10	1.4416 (10)	C22—H22A	0.9500
C9—H9A	0.9500	C23—C24	1.3937 (12)
C10—C12	1.3886 (10)	C23—H23A	0.9500
C10—C11	1.4305 (10)	C24—H24A	0.9500
C12—N1—N2	111.99 (6)	N1—C12—H12A	126.2
C12—N1—C19	127.99 (6)	C10—C12—H12A	126.2
N2—N1—C19	119.98 (6)	C18—C13—C14	119.08 (7)
C11—N2—N1	105.17 (6)	C18—C13—C11	120.35 (7)
C2—C1—C6	120.43 (7)	C14—C13—C11	120.39 (7)
C2—C1—H1A	119.8	C15—C14—C13	120.62 (7)
C6—C1—H1A	119.8	C15—C14—H14A	119.7
C3—C2—C1	120.10 (7)	C13—C14—H14A	119.7
C3—C2—H2A	119.9	C14—C15—C16	119.86 (8)
C1—C2—H2A	119.9	C14—C15—H15A	120.1
C4—C3—C2	119.96 (7)	C16—C15—H15A	120.1
C4—C3—H3A	120.0	C17—C16—C15	119.82 (7)
C2—C3—H3A	120.0	C17—C16—H16A	120.1
C3—C4—C5	120.16 (8)	C15—C16—H16A	120.1
C3—C4—H4A	119.9	C16—C17—C18	120.51 (7)
C5—C4—H4A	119.9	C16—C17—H17A	119.7
C4—C5—C6	120.30 (7)	C18—C17—H17A	119.7
C4—C5—H5A	119.8	C17—C18—C13	120.11 (7)
C6—C5—H5A	119.8	C17—C18—H18A	119.9
C5—C6—C1	119.04 (7)	C13—C18—H18A	119.9
C5—C6—C7	122.63 (7)	C24—C19—C20	120.83 (7)
C1—C6—C7	118.34 (6)	C24—C19—N1	119.87 (7)
O1—C7—C8	121.76 (7)	C20—C19—N1	119.30 (7)
O1—C7—C6	119.81 (7)	C19—C20—C21	119.29 (8)
C8—C7—C6	118.43 (6)	C19—C20—H20A	120.4
C9—C8—C7	120.44 (7)	C21—C20—H20A	120.4
C9—C8—H8A	119.8	C22—C21—C20	120.50 (8)
C7—C8—H8A	119.8	C22—C21—H21A	119.7
C8—C9—C10	128.27 (7)	C20—C21—H21A	119.7
C8—C9—H9A	115.9	C23—C22—C21	119.52 (8)
C10—C9—H9A	115.9	C23—C22—H22A	120.2
C12—C10—C11	103.95 (6)	C21—C22—H22A	120.2
C12—C10—C9	123.14 (7)	C22—C23—C24	120.88 (8)
C11—C10—C9	132.89 (7)	C22—C23—H23A	119.6
N2—C11—C10	111.32 (6)	C24—C23—H23A	119.6
N2—C11—C13	117.90 (6)	C19—C24—C23	118.96 (8)
C10—C11—C13	130.69 (7)	C19—C24—H24A	120.5
N1—C12—C10	107.56 (6)	C23—C24—H24A	120.5
C12—N1—N2—C11	0.28 (8)	C11—C10—C12—N1	0.79 (8)
C19—N1—N2—C11	178.30 (7)	C9—C10—C12—N1	-178.05 (7)
C6—C1—C2—C3	-0.03 (13)	N2—C11—C13—C18	-47.06 (10)

C1—C2—C3—C4	0.94 (13)	C10—C11—C13—C18	136.80 (8)
C2—C3—C4—C5	-1.00 (14)	N2—C11—C13—C14	128.07 (8)
C3—C4—C5—C6	0.15 (14)	C10—C11—C13—C14	-48.06 (11)
C4—C5—C6—C1	0.76 (12)	C18—C13—C14—C15	0.52 (11)
C4—C5—C6—C7	-179.03 (8)	C11—C13—C14—C15	-174.68 (7)
C2—C1—C6—C5	-0.82 (12)	C13—C14—C15—C16	-0.10 (12)
C2—C1—C6—C7	178.98 (7)	C14—C15—C16—C17	-0.59 (12)
C5—C6—C7—O1	-162.50 (8)	C15—C16—C17—C18	0.85 (12)
C1—C6—C7—O1	17.72 (11)	C16—C17—C18—C13	-0.43 (12)
C5—C6—C7—C8	17.37 (11)	C14—C13—C18—C17	-0.26 (11)
C1—C6—C7—C8	-162.41 (7)	C11—C13—C18—C17	174.95 (7)
O1—C7—C8—C9	6.89 (12)	C12—N1—C19—C24	-10.42 (12)
C6—C7—C8—C9	-172.98 (7)	N2—N1—C19—C24	171.91 (7)
C7—C8—C9—C10	-179.26 (7)	C12—N1—C19—C20	169.10 (8)
C8—C9—C10—C12	171.25 (8)	N2—N1—C19—C20	-8.57 (11)
C8—C9—C10—C11	-7.21 (14)	C24—C19—C20—C21	-0.83 (12)
N1—N2—C11—C10	0.25 (8)	N1—C19—C20—C21	179.65 (7)
N1—N2—C11—C13	-176.60 (6)	C19—C20—C21—C22	0.74 (13)
C12—C10—C11—N2	-0.66 (9)	C20—C21—C22—C23	0.16 (13)
C9—C10—C11—N2	178.01 (8)	C21—C22—C23—C24	-1.00 (14)
C12—C10—C11—C13	175.68 (8)	C20—C19—C24—C23	0.02 (13)
C9—C10—C11—C13	-5.65 (14)	N1—C19—C24—C23	179.53 (8)
N2—N1—C12—C10	-0.70 (9)	C22—C23—C24—C19	0.91 (14)
C19—N1—C12—C10	-178.53 (7)		

Hydrogen-bond geometry (\AA , $^\circ$)

Cg2 and Cg3 are the centroids of the C20—C25 and C13—C18 rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C12—H12A \cdots O1 ⁱ	0.95	2.27	3.2019 (11)	167
C15—H15A \cdots Cg2 ⁱⁱ	0.95	2.81	3.6171 (9)	143
C2—H2A \cdots Cg3 ⁱⁱⁱ	0.95	2.63	3.4304 (9)	143

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