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2-Methoxy-4-[3-(3-nitrophenyl)-4,5-dihydro-1H-pyrazol-5-yl]phenol

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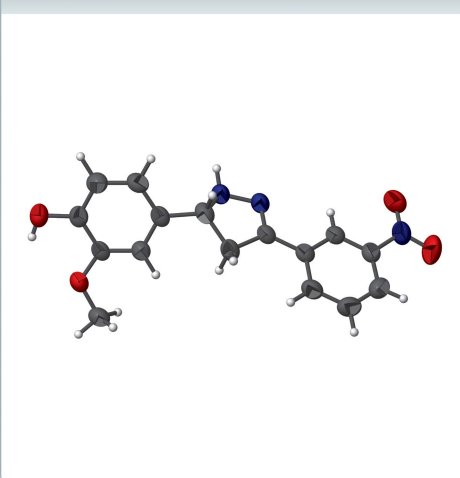
Keywords: crystal structure; 1H-pyrazole; chalcones; hydrogen bonding.

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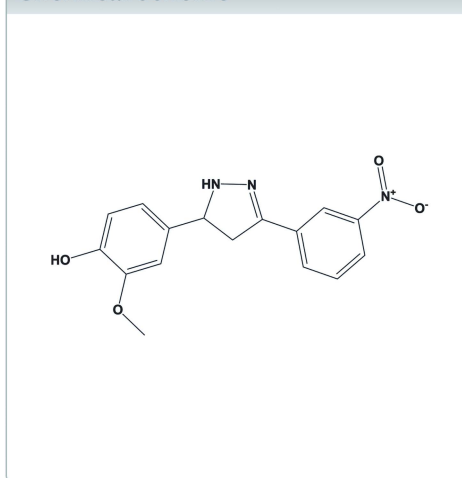
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, C₁₆H₁₅N₃O₄, the pyrazole ring has an envelope conformation, with the C atom substituted by the 2-methoxyphenol ring as the flap. Its mean plane makes dihedral angles of 56.78 (9) and 9.7 (1)° with the 2-methoxyphenol and 3-nitrophenyl rings, respectively. The benzene rings are inclined to one another by 49.37 (8)°. In the crystal, molecules are linked by pairs of O—H...N hydrogen bonds, forming inversion dimers with an R₂²(16) ring motif. The dimers are linked by C—H...O hydrogen bonds, forming slabs parallel to the *ac* plane. There are slipped parallel π – π interactions present within the slabs, involving inversion-related 2-methoxyphenol rings [intercentroid distance = 3.729 (1) Å] and inversion-related 3-nitrophenyl rings [intercentroid distance = 3.831 (1) Å].

3D view



Chemical scheme



Structure description

Pyrazoles and their derivatives have significant importance as biological agents and play a vital role in drug discovery. Pyrazoles have been widely exploited for their antitumor (Sankappa Rai *et al.*, 2015), antibacterial and antifungal, antiviral, antiparasitic, anti-inflammatory, anti-diabetic, anaesthetic and analgesic properties and their anti-tubercular (Gupta & Kaskhedikar, 2013) and insecticidal activities (Hamada & Abdo, 2015). Chalcones have played a crucial role in the development of heterocyclic compounds, and they form the skeleton for pyrazole synthesis. A classical synthesis of pyrazole involves nucleophilic addition of ketones and aldehydes in presence of a base-like KOH to follow aldol condensation (Hamada & Abdo, 2015) and yield α,β -unsaturated ketones (chalcones), which undergo a subsequent cyclization reaction with hydrazine hydrate to afford

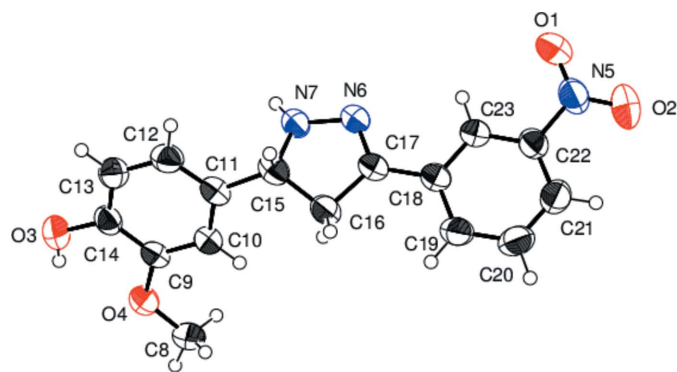


Figure 1
The molecular structure of the title compound, showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

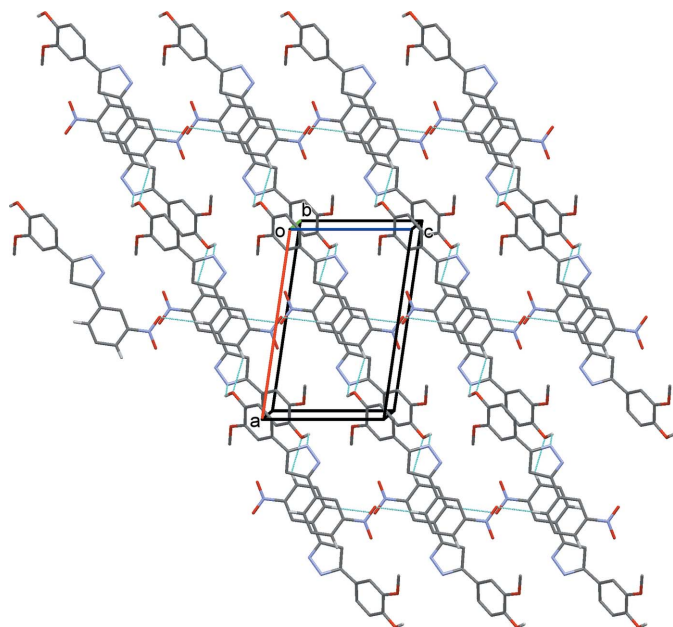


Figure 2
The crystal packing of the title compound viewed along the *a* axis. Hydrogen bonds are shown as dashed lines (see Table 1) and H atoms not involved in these interactions are omitted for clarity.

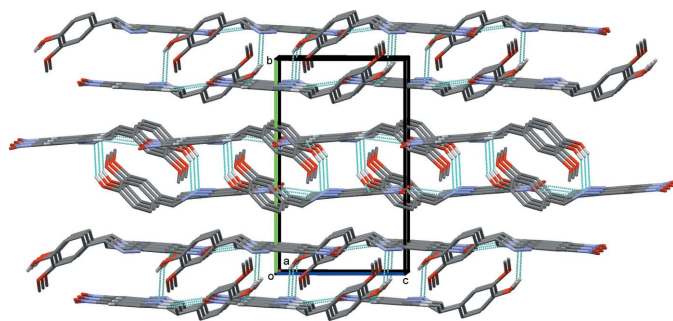


Figure 3
The crystal packing of the title compound viewed along the *b* axis. Hydrogen bonds are shown as dashed lines (see Table 1) and H atoms not involved in these interactions are omitted for clarity.

Table 1
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>
O3—H3···N7 ⁱ	0.82	2.31	2.863 (2)	126
C19—H19···O1 ⁱⁱ	0.95 (2)	2.57 (2)	3.510 (2)	168.0 (16)
C21—H21···O3 ⁱⁱⁱ	0.91 (2)	2.60 (2)	3.330 (2)	137.8 (19)

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

pyrazoles. In an effort to evaluate the antitubercular activity of vanillin-based pyrazoles, we report herein on the synthesis and crystal structural of the title pyrazole derivative.

The molecular structure of the title compound is shown in Fig. 1. The pyrazole ring (N6/N6/C15–C17) has an envelope conformation with atom C15 as the flap. The benzene rings (C19–C14) and (C18–C23) are inclined to the mean plane of the pyrazole ring by 56.78 (9) and 9.7 (1)°, respectively, and to each other by 49.37 (8)°.

In the crystal, molecules are linked *via* pairs of O—H···N hydrogen bonds, forming inversion dimers with an $R_2^2(16)$ ring motif (Table 1 and Fig. 2). The dimers are linked *via* C—H···O hydrogen bonds, forming slabs parallel to the *ac* plane (Table 1 and Fig. 3). Within the slabs, there are slipped parallel π – π interactions present involving inversion-related 2-meth-

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{15}N_3O_4$
M_r	313.31
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
<i>a</i> , <i>b</i> , <i>c</i> (Å)	13.1432 (11), 13.6130 (12), 8.3381 (7)
β (°)	98.495 (4)
<i>V</i> (Å ³)	1475.5 (2)
<i>Z</i>	4
Radiation type	Cu $K\alpha$
μ (mm ⁻¹)	0.86
Crystal size (mm)	0.24 × 0.20 × 0.12
Data collection	
Diffractometer	Bruker SMART CCD area-detector
Absorption correction	Multi-scan (SADABS; Bruker, 2001)
T_{min} , T_{max}	0.770, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12553, 2436, 2094
R_{int}	0.041
($\sin \theta/\lambda$) _{max} (Å ⁻¹)	0.586
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, <i>S</i>	0.039, 0.113, 1.00
No. of reflections	2436
No. of parameters	264
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å ⁻³)	0.23, -0.22

Computer programs: SMART and SAINT (Bruker, 2001), SHELXS97 (Sheldrick, 2008), SHELXL2014 (Sheldrick, 2015), ORTEP-3 for Windows (Farrugia, 2012), Mercury (Macrae *et al.*, 2008), and PLATON (Spek, 2009).

oxyphenol rings [$Cg2 \cdots Cg2^i = 3.729$ (1) Å, $Cg2$ is the centroid of ring C9–C14, interplanar distance = 3.377 (1) Å, slippage = 1.583 Å, symmetry code: (i) $-x, -y + 1, -z$], and inversion-related 3-nitrophenyl rings [$Cg3 \cdots Cg3^{ii} = 3.831$ (1) Å, $Cg3$ is the centroid of ring C18–C23, interplanar distance = 3.356 (1) Å, slippage = 1.404 Å, symmetry code: (ii) $-x + 1, -y + 1, -z + 1$].

Synthesis and crystallization

To a solution of vanillin (1 mmol) and 3-nitroacetophenone (1 mmol) in absolute alcohol (25 ml) an ethanol solution of KOH (0.282 g, 10.088 mmol) was added at 298–300 K. The reaction mixture was stirred at room temperature and the progress of the reaction was monitored by TLC, using hexane: ethyl acetate (8:2). After the completion of reaction (24 h), the reaction mixture was poured into ice cold water (100 ml) and neutralized with dilute HCL. The precipitate obtained was recrystallized in ethanol. The chalcone product (1 mmol) and hydrazine hydrate (4 mmol) were dissolved in absolute alcohol (20 ml) and refluxed for 9–10 h. The reaction mixture was poured into crushed ice and stirred, the solid thus obtained was filtered off and washed with cold water, dried and recrystallized in ethanol giving colourless prismatic crystal (yield 65%). Spectroscopic data: IR (KBr disk, cm^{-1}) 3364 (OH), 3310 (NH), 2965 (C–H), 1592 (Ar–C=C), 1513 (*asym*, Ar–NO₂), 1340 (*sym*, Ar–NO₂), 1260 (–OCH₃); ¹H NMR (CDCl₃, δ p.p.m.): 8.92 (*s*, 1H, NH), 9.92 (*s*, 1H, OH), 6.96–7.64 (*m*, 7H, Ar–H), 6.8 (*t*, 1H, CH–C5), 4.72 (*d*, 2H, CH₂), 3.84 (*s*, 3H, OCH₃); ¹³C NMR (CDCl₃, δ p.p.m.): 148–119 (12C, Ar–

C), 110.67 (1C, C), 62.4 (1C, CH), 59.56 (1C, CH₂), 48.86 (1C, OCH₃); LC–MS *m/z*: 314.1 (M^{+1} 100%), Elemental analysis for C₁₆H₁₅N₃O₄: found C, 61.34; H, 4.83; N, 13.41; O, 20.43%. calc. C, 61.31; H, 4.76; N, 13.44; O, 20.42%.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x160466 [doi:10.1107/S2414314616004661]

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Crystal data

$C_{16}H_{15}N_3O_4$

$M_r = 313.31$

Monoclinic, $P2_1/c$

$a = 13.1432$ (11) Å

$b = 13.6130$ (12) Å

$c = 8.3381$ (7) Å

$\beta = 98.495$ (4)°

$V = 1475.5$ (2) Å³

$Z = 4$

$F(000) = 656$

$D_x = 1.410$ Mg m⁻³

Melting point: 300 K

Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å

Cell parameters from 2436 reflections

$\theta = 4.7$ – 64.5 °

$\mu = 0.86$ mm⁻¹

$T = 296$ K

Prism, colourless

$0.24 \times 0.20 \times 0.12$ mm

Data collection

Bruker SMART CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

ω and φ scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2001)

$T_{\min} = 0.770$, $T_{\max} = 1.000$

12553 measured reflections

2436 independent reflections

2094 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.041$

$\theta_{\max} = 64.5$ °, $\theta_{\min} = 4.7$ °

$h = -15 \rightarrow 15$

$k = -15 \rightarrow 15$

$l = -7 \rightarrow 9$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.039$

$wR(F^2) = 0.113$

$S = 1.00$

2436 reflections

264 parameters

0 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: mixed

H atoms treated by a mixture of independent
and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0633P)^2 + 0.3151P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.23$ e Å⁻³

$\Delta\rho_{\min} = -0.22$ e Å⁻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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.47950 (12)	0.38474 (13)	1.00496 (16)	0.0866 (5)
O2	0.64242 (13)	0.39816 (17)	1.0087 (2)	0.1116 (6)
O3	-0.12236 (9)	0.41880 (10)	-0.30456 (14)	0.0649 (4)
H3	-0.1027	0.4622	-0.3609	0.097*
O4	0.06043 (9)	0.50817 (9)	-0.28614 (13)	0.0600 (3)
N5	0.55509 (13)	0.38872 (12)	0.93716 (19)	0.0696 (4)
N6	0.24426 (10)	0.37549 (11)	0.49118 (16)	0.0555 (4)
N7	0.15583 (11)	0.37666 (12)	0.37290 (16)	0.0574 (4)
C8	0.15531 (15)	0.55902 (15)	-0.2786 (2)	0.0599 (5)
C9	0.05066 (11)	0.44201 (11)	-0.16650 (17)	0.0457 (4)
C10	0.12593 (12)	0.41954 (12)	-0.03695 (18)	0.0481 (4)
C11	0.10725 (12)	0.34898 (11)	0.07692 (18)	0.0484 (4)
C12	0.01357 (13)	0.30044 (13)	0.0551 (2)	0.0548 (4)
C13	-0.06238 (13)	0.32419 (13)	-0.0724 (2)	0.0550 (4)
C14	-0.04530 (12)	0.39581 (12)	-0.18145 (18)	0.0491 (4)
C15	0.18282 (13)	0.32519 (13)	0.22660 (18)	0.0527 (4)
C16	0.29462 (13)	0.35523 (15)	0.23767 (19)	0.0528 (4)
C17	0.32268 (12)	0.36558 (11)	0.41811 (18)	0.0467 (4)
C18	0.42759 (12)	0.36985 (11)	0.50882 (19)	0.0469 (4)
C19	0.51340 (14)	0.36513 (13)	0.4293 (2)	0.0578 (4)
C20	0.61173 (15)	0.36814 (15)	0.5153 (3)	0.0682 (5)
C21	0.62715 (15)	0.37541 (14)	0.6818 (3)	0.0640 (5)
C22	0.54125 (13)	0.38058 (12)	0.7590 (2)	0.0537 (4)
C23	0.44264 (13)	0.37823 (12)	0.6769 (2)	0.0492 (4)
H8A	0.1453 (15)	0.6004 (15)	-0.375 (3)	0.075 (6)*
H8B	0.1670 (15)	0.6010 (15)	-0.177 (3)	0.069 (5)*
H8C	0.2140 (16)	0.5119 (15)	-0.281 (2)	0.074 (6)*
H10	0.1931 (13)	0.4536 (13)	-0.027 (2)	0.055 (4)*
H12	0.0020 (14)	0.2500 (14)	0.131 (2)	0.065 (5)*
H13	-0.1337 (14)	0.2891 (13)	-0.083 (2)	0.062 (5)*
H15	0.1804 (14)	0.2515 (15)	0.249 (2)	0.067 (5)*
H16A	0.3339 (15)	0.3090 (15)	0.188 (2)	0.069 (5)*
H16B	0.3027 (14)	0.4186 (16)	0.188 (2)	0.067 (5)*
H19	0.5030 (15)	0.3598 (14)	0.314 (3)	0.072 (6)*
H20	0.6710 (17)	0.3609 (15)	0.457 (3)	0.080 (6)*
H21	0.6912 (18)	0.3768 (15)	0.741 (3)	0.081 (7)*
H23	0.3874 (15)	0.3834 (13)	0.729 (2)	0.063 (5)*
H7	0.1015 (17)	0.3524 (15)	0.413 (3)	0.076 (6)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0900 (11)	0.1241 (13)	0.0460 (7)	-0.0160 (9)	0.0117 (7)	0.0019 (7)
O2	0.0804 (10)	0.1741 (18)	0.0700 (10)	-0.0177 (10)	-0.0230 (8)	-0.0032 (10)
O3	0.0575 (7)	0.0804 (8)	0.0524 (7)	-0.0051 (6)	-0.0067 (5)	0.0029 (6)

O4	0.0588 (7)	0.0743 (8)	0.0453 (6)	-0.0031 (5)	0.0028 (5)	0.0145 (5)
N5	0.0723 (10)	0.0803 (11)	0.0516 (9)	-0.0099 (8)	-0.0066 (8)	0.0043 (7)
N6	0.0522 (8)	0.0750 (9)	0.0393 (7)	-0.0001 (6)	0.0061 (6)	0.0035 (6)
N7	0.0499 (8)	0.0837 (10)	0.0383 (7)	-0.0016 (7)	0.0061 (6)	0.0030 (7)
C8	0.0628 (11)	0.0688 (12)	0.0501 (10)	-0.0031 (9)	0.0152 (8)	0.0092 (9)
C9	0.0539 (8)	0.0501 (9)	0.0338 (8)	0.0037 (7)	0.0088 (6)	0.0002 (6)
C10	0.0503 (8)	0.0539 (9)	0.0404 (8)	-0.0007 (7)	0.0071 (7)	-0.0013 (7)
C11	0.0577 (9)	0.0504 (9)	0.0372 (8)	0.0039 (7)	0.0071 (7)	-0.0003 (6)
C12	0.0647 (10)	0.0526 (9)	0.0484 (9)	-0.0046 (8)	0.0128 (8)	0.0044 (7)
C13	0.0570 (9)	0.0573 (10)	0.0508 (9)	-0.0061 (8)	0.0080 (8)	-0.0044 (8)
C14	0.0534 (9)	0.0543 (9)	0.0390 (8)	0.0016 (7)	0.0041 (7)	-0.0081 (7)
C15	0.0649 (10)	0.0511 (9)	0.0412 (8)	0.0012 (8)	0.0049 (7)	0.0046 (7)
C16	0.0562 (9)	0.0622 (11)	0.0399 (9)	0.0087 (8)	0.0070 (7)	0.0004 (8)
C17	0.0540 (9)	0.0477 (8)	0.0387 (8)	0.0022 (6)	0.0081 (7)	0.0047 (6)
C18	0.0528 (9)	0.0451 (8)	0.0430 (8)	0.0010 (6)	0.0085 (7)	0.0044 (6)
C19	0.0612 (10)	0.0660 (11)	0.0485 (10)	0.0005 (8)	0.0158 (8)	0.0066 (8)
C20	0.0551 (10)	0.0825 (13)	0.0710 (13)	-0.0003 (9)	0.0225 (9)	0.0084 (10)
C21	0.0501 (10)	0.0712 (12)	0.0691 (12)	-0.0045 (8)	0.0034 (9)	0.0087 (9)
C22	0.0570 (9)	0.0562 (9)	0.0462 (9)	-0.0052 (7)	0.0022 (7)	0.0063 (7)
C23	0.0512 (9)	0.0532 (9)	0.0437 (9)	-0.0022 (7)	0.0091 (7)	0.0045 (7)

Geometric parameters (Å, °)

O1—N5	1.215 (2)	C12—C13	1.384 (2)
O2—N5	1.219 (2)	C12—H12	0.96 (2)
O3—C14	1.3676 (19)	C13—C14	1.374 (2)
O3—H3	0.8200	C13—H13	1.045 (18)
O4—C9	1.3640 (18)	C15—C16	1.515 (2)
O4—C8	1.419 (2)	C15—H15	1.02 (2)
N5—C22	1.474 (2)	C16—C17	1.502 (2)
N6—C17	1.280 (2)	C16—H16A	0.95 (2)
N6—N7	1.409 (2)	C16—H16B	0.97 (2)
N7—C15	1.494 (2)	C17—C18	1.473 (2)
N7—H7	0.89 (2)	C18—C23	1.390 (2)
C8—H8A	0.98 (2)	C18—C19	1.392 (2)
C8—H8B	1.02 (2)	C19—C20	1.383 (3)
C8—H8C	1.01 (2)	C19—H19	0.95 (2)
C9—C10	1.387 (2)	C20—C21	1.377 (3)
C9—C14	1.398 (2)	C20—H20	0.98 (2)
C10—C11	1.398 (2)	C21—C22	1.381 (3)
C10—H10	0.990 (17)	C21—H21	0.91 (2)
C11—C12	1.385 (2)	C22—C23	1.374 (2)
C11—C15	1.511 (2)	C23—H23	0.902 (19)
C14—O3—H3	109.5	N7—C15—C11	111.56 (13)
C9—O4—C8	117.81 (13)	N7—C15—C16	99.72 (13)
O1—N5—O2	123.54 (17)	C11—C15—C16	120.38 (14)
O1—N5—C22	118.55 (15)	N7—C15—H15	107.2 (10)

O2—N5—C22	117.90 (18)	C11—C15—H15	109.0 (11)
C17—N6—N7	107.88 (13)	C16—C15—H15	108.1 (10)
N6—N7—C15	107.18 (12)	C17—C16—C15	100.30 (13)
N6—N7—H7	110.9 (13)	C17—C16—H16A	115.4 (12)
C15—N7—H7	115.4 (14)	C15—C16—H16A	112.4 (11)
O4—C8—H8A	103.6 (12)	C17—C16—H16B	108.5 (11)
O4—C8—H8B	109.6 (11)	C15—C16—H16B	112.4 (11)
H8A—C8—H8B	110.5 (16)	H16A—C16—H16B	107.8 (16)
O4—C8—H8C	111.0 (11)	N6—C17—C18	120.68 (14)
H8A—C8—H8C	111.3 (16)	N6—C17—C16	113.02 (14)
H8B—C8—H8C	110.7 (16)	C18—C17—C16	126.23 (14)
O4—C9—C10	125.58 (14)	C23—C18—C19	118.64 (16)
O4—C9—C14	114.39 (13)	C23—C18—C17	120.26 (14)
C10—C9—C14	120.03 (14)	C19—C18—C17	121.10 (15)
C9—C10—C11	120.27 (15)	C20—C19—C18	120.82 (17)
C9—C10—H10	119.1 (10)	C20—C19—H19	120.6 (12)
C11—C10—H10	120.6 (10)	C18—C19—H19	118.6 (12)
C12—C11—C10	118.71 (15)	C21—C20—C19	120.82 (18)
C12—C11—C15	117.99 (14)	C21—C20—H20	119.7 (13)
C10—C11—C15	123.26 (15)	C19—C20—H20	119.3 (13)
C11—C12—C13	121.03 (16)	C20—C21—C22	117.69 (18)
C11—C12—H12	118.5 (11)	C20—C21—H21	122.3 (14)
C13—C12—H12	120.4 (11)	C22—C21—H21	120.0 (14)
C14—C13—C12	120.26 (16)	C23—C22—C21	122.83 (17)
C14—C13—H13	120.1 (10)	C23—C22—N5	118.12 (16)
C12—C13—H13	119.6 (10)	C21—C22—N5	119.05 (16)
O3—C14—C13	118.94 (14)	C22—C23—C18	119.19 (15)
O3—C14—C9	121.48 (14)	C22—C23—H23	121.6 (12)
C13—C14—C9	119.56 (14)	C18—C23—H23	119.2 (12)
C17—N6—N7—C15	23.48 (17)	C11—C15—C16—C17	152.25 (15)
C8—O4—C9—C10	-0.2 (2)	N7—N6—C17—C18	175.02 (13)
C8—O4—C9—C14	179.31 (15)	N7—N6—C17—C16	-2.02 (19)
O4—C9—C10—C11	-178.96 (14)	C15—C16—C17—N6	-19.28 (19)
C14—C9—C10—C11	1.6 (2)	C15—C16—C17—C18	163.88 (14)
C9—C10—C11—C12	1.7 (2)	N6—C17—C18—C23	4.3 (2)
C9—C10—C11—C15	-176.05 (14)	C16—C17—C18—C23	-179.11 (16)
C10—C11—C12—C13	-3.1 (2)	N6—C17—C18—C19	-176.06 (15)
C15—C11—C12—C13	174.84 (15)	C16—C17—C18—C19	0.6 (2)
C11—C12—C13—C14	1.0 (3)	C23—C18—C19—C20	0.4 (2)
C12—C13—C14—O3	-178.94 (14)	C17—C18—C19—C20	-179.32 (16)
C12—C13—C14—C9	2.4 (2)	C18—C19—C20—C21	0.3 (3)
O4—C9—C14—O3	-1.8 (2)	C19—C20—C21—C22	-0.7 (3)
C10—C9—C14—O3	177.69 (14)	C20—C21—C22—C23	0.4 (3)
O4—C9—C14—C13	176.82 (14)	C20—C21—C22—N5	-179.81 (17)
C10—C9—C14—C13	-3.7 (2)	O1—N5—C22—C23	6.1 (2)
N6—N7—C15—C11	-162.14 (14)	O2—N5—C22—C23	-174.65 (18)
N6—N7—C15—C16	-33.87 (16)	O1—N5—C22—C21	-173.77 (18)

C12—C11—C15—N7	-79.11 (19)	O2—N5—C22—C21	5.5 (3)
C10—C11—C15—N7	98.68 (18)	C21—C22—C23—C18	0.3 (3)
C12—C11—C15—C16	164.65 (16)	N5—C22—C23—C18	-179.53 (14)
C10—C11—C15—C16	-17.5 (2)	C19—C18—C23—C22	-0.6 (2)
N7—C15—C16—C17	30.07 (15)	C17—C18—C23—C22	179.03 (14)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O3—H3 \cdots N7 ⁱ	0.82	2.31	2.863 (2)	126
C19—H19 \cdots O1 ⁱⁱ	0.95 (2)	2.57 (2)	3.510 (2)	168.0 (16)
C21—H21 \cdots O3 ⁱⁱⁱ	0.91 (2)	2.60 (2)	3.330 (2)	137.8 (19)

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