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Crystal structure of (2-hydroxy-5-methylphenyl)(3-methyl-1-phenyl-1*H*-pyrazolo[3,4-*b*]pyridin-5-yl)methanone

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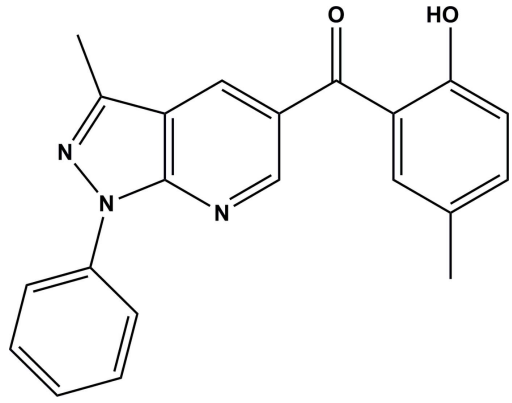
In the title compound, $C_{21}H_{17}N_3O_2$, the 2-hydroxy-5-methylphenyl ring and the phenyl ring are inclined to the mean plane of the pyrazolopyridine moiety (r.m.s. deviation = 0.013 Å) by 52.89 (9) and 19.63 (8)°, respectively, and to each other by 42.83 (11)°. In the molecule, there are intramolecular O—H···O and C—H···N hydrogen bonds, both enclosing an *S*(6) ring motif. In the crystal, molecules stack along the *c*-axis direction, forming columns within which there are a number of π–π interactions [the inter-centroid distances vary from 3.5278 (10) to 3.8625 (10) Å]. The columns are linked by C—H···π interactions, forming slabs parallel to (100).

Keywords: crystal structure; pyrazoles; propenones; pyrazolopyridine; intramolecular hydrogen bonding; π–π interactions; C—H···π interactions.

CCDC reference: 1406889

1. Related literature

For some details of the biological activity of pyrazole derivatives, see: Burger & Iorio (1979, 1980); Kalluraya & Ramesh (2001); Windholz (2003). For the antibacterial activity of propenones, see: Holla *et al.* (1994). For details of the pyrazole moiety found in blockbuster drugs, see: Penning *et al.* (1997) for celecobix; Terrett *et al.* (1996) for sildenafil; Seltzman *et al.* (1995) for rimonabant.



2. Experimental

2.1. Crystal data

$C_{21}H_{17}N_3O_2$
M_r = 343.38
Monoclinic, $P2_1/c$
a = 14.7164 (7) Å
b = 16.7306 (9) Å
c = 7.0733 (3) Å
β = 94.857 (2)°
V = 1735.29 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 K
0.25 × 0.20 × 0.20 mm

2.2. Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.979, T_{max} = 0.983
10536 measured reflections
3055 independent reflections
2001 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.125
S = 1.04
3055 reflections
237 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

*Cg*3 and *Cg*4 are the centroids of rings C1–C4/C6/C7 and C16–C21, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2	0.82	1.91	2.613 (2)	143
C21—H21···N1	0.93	2.41	3.019 (3)	123
C5—H5*A*···*Cg*3^{i}	0.96	2.97	3.703 (3)	134
C20—H20···*Cg*4^{i}	0.93	2.80	3.608 (2)	146

Symmetry code: (i) $x, -y+\frac{1}{2}, z-\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); 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: *SHELXL97* and *PLATON* (Spek, 2009).

Acknowledgements

The authors thank the Department of Chemistry, IIT, Chennai, India, for the X-ray intensity data collection.

Supporting information for this paper is available from the IUCr electronic archives (Reference: SU5154).

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supporting information

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Crystal structure of (2-hydroxy-5-methylphenyl)(3-methyl-1-phenyl-1*H*-pyrazolo[3,4-*b*]pyridin-5-yl)methanone

Rajamani Raja, Nataraj Poomathi, Paramasivam T. Perumal and A. SubbiahPandi

S1. Comments

Pyrazole derivatives are reported to possess varied biological activities such as anti-inflammatory (Windholz, 2003), analgesic (Windholz, 2003), hypoglysemic, seditive (Burger *et al.*, 1979), hypnotic (Burger *et al.*, 1980), antifungal and antibacterial (Kalluraya & Ramesh, 2001) activities. Propenones are also found to show good antibacterial activity (Holla *et al.*, 1994). The pyrazole moiety is found in blockbuster drugs such as celecobix (Penning *et al.*, 1997), sildenafil (Terrett *et al.*, 1996) and rimonabant (Seltzmann *et al.*, 1995).

The molecular structure of the title molecule is shown in Fig. 1. The 2-hydroxy-5-methylphenyl ring (C1—C4/C6/C7) and the phenyl ring (C16—C21) are inclined to the mean plane of the pyrazolopyridine moiety (N1—N3/C9—C14; r.m.s. deviation = 0.013 Å) by 52.89 (9) and 19.63 (8) °, respectively, and to each other by 42.83 (11) °. The molecular conformation is partly determined by the intramolecular O—H···O hydrogen bond with an S(6) ring motif, and a C—H···N short contact enclosing a second S(6) ring motif (Table 1 and Fig. 1).

In the crystal, the molecules stack along the *c* axis direction forming columns, within which there are a number of *π*–*π* interactions [Cg1···Cg1^{i} = 3.7660 (10) Å, interplanar distance = 3.4748 (7) Å, slippage = 1.452 Å; Cg1··· Cg1^{ii} = 3.5278 (10) Å, interplanar distance = 3.4477 (7) Å, slippage = 0.747 Å; Cg1···Cg2^{i} = 3.6162 (10) Å; Cg1···Cg2^{ii} = 3.8625 (10) Å; Cg1 and Cg2 are the centroids of rings N2/N3/C11—C14 and N1/C9—C13, respectively; symmetry codes: (i) -x + 1, -y, -z; (ii) -x + 1, -y, -z + 1]. The columns are linked by C—H···*π* interactions (Table 1 and Fig. 2) forming slabs parallel to (100).

S2. Synthesis and crystallization

To a mixture of 3-formylchromone and 5-amino-3-methyl-1-phenyl pyrazole in ethanol, was added a catalytic amount of $In(OTf)_3$ and the resulting mixture was refluxed for ca. 20 min. The precipitate formed was filtered and dried under vacuum to afford the pure title product (yield: 87%). It was recrystallized from ethanol and DMSO-D_6 by slow evaporation over 48 h, giving colourless block-like crystals.

S3. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The O- and C-bound H atoms were positioned geometrically and allowed to ride on their parent atoms: O—H = 0.82 Å, C–H = 0.93–0.96 Å with U_{iso}(H) = 1.5U_{eq}(O,C) for the hydroxyl and methyl H atoms and 1.2U_{eq}(C) for other H atoms.

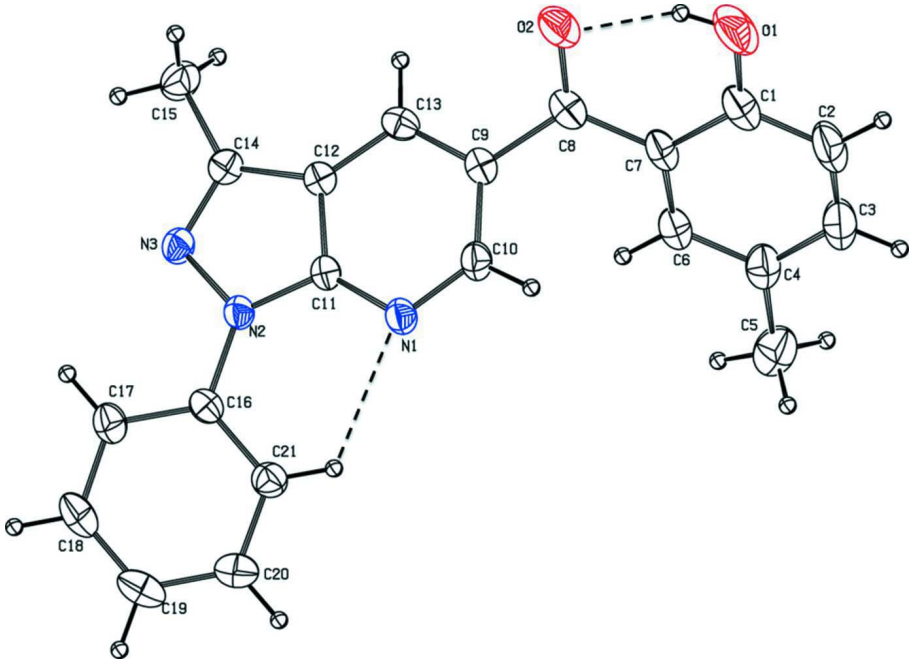

Figure 1

The molecular structure of the title compound, with atom labelling. Displacement ellipsoids are drawn at the 30% probability level. Intramolecular hydrogen bonds are shown as dashed lines (see Table 1 for details)

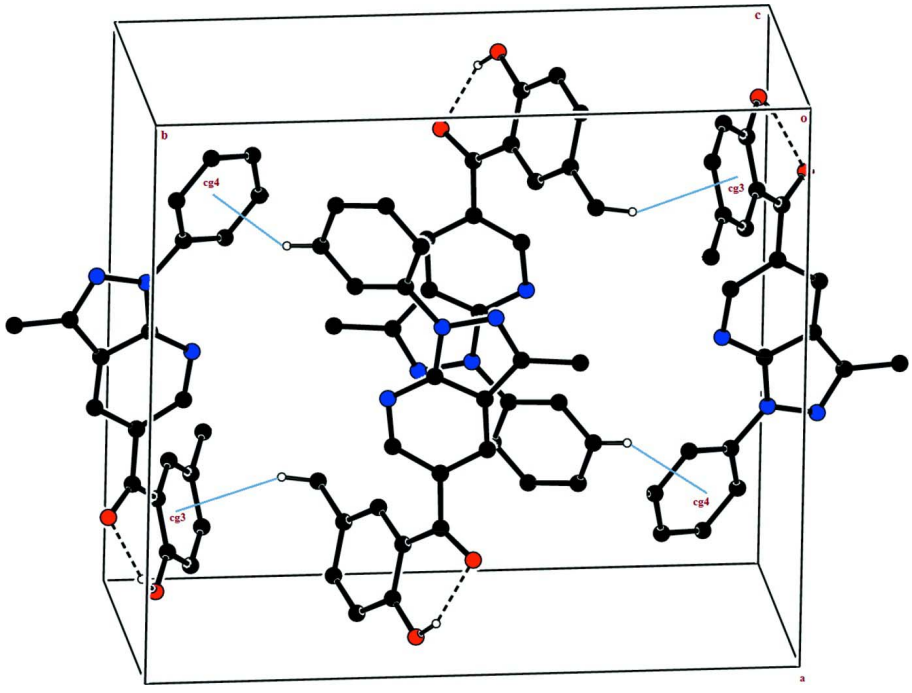

Figure 2

The crystal packing of the title compound, viewed along the *c* axis. The O—H···O and C—H···π interactions are shown as dashed lines (see Table 1 for details).

(2-Hydroxy-5-methylphenyl)(3-methyl-1-phenyl-1*H*-pyrazolo[3,4-*b*]pyridin-5-yl)methanone

Crystal data

$C_{21}H_{17}N_3O_2$
M_r = 343.38
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 14.7164 (7) Å
b = 16.7306 (9) Å
c = 7.0733 (3) Å
β = 94.857 (2)°
V = 1735.29 (14) Å^3
Z = 4
$F(000)$ = 720
D_x = 1.314 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2001 reflections
θ = 1.4–25.0°
μ = 0.09 mm^{-1}
T = 293 K
Block, colourless
0.25 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.979, T_{max} = 0.983
10536 measured reflections
3055 independent reflections
2001 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 25.0°, θ_{min} = 1.4°
h = −17→17
k = −19→19
l = −5→8

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.125
S = 1.04
3055 reflections
237 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
$w = 1/[\sigma^2(F_o^2) + (0.0597P)^2 + 0.1547P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 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.

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
C1	0.05588 (15)	0.09390 (16)	0.0431 (4)	0.0621 (7)
C2	0.00532 (16)	0.13878 (17)	−0.0938 (4)	0.0746 (8)
H2	−0.0552	0.1509	−0.0781	0.090*
C3	0.04416 (17)	0.16526 (16)	−0.2520 (4)	0.0724 (8)

H3	0.0090	0.1950	−0.3420	0.087*
C4	0.13449 (15)	0.14903 (14)	−0.2816 (3)	0.0559 (6)
C5	0.17618 (19)	0.17799 (17)	−0.4560 (4)	0.0787 (8)
H5A	0.1872	0.2344	−0.4458	0.118*
H5B	0.1352	0.1674	−0.5660	0.118*
H5C	0.2328	0.1506	−0.4675	0.118*
C6	0.18475 (14)	0.10574 (13)	−0.1436 (3)	0.0491 (6)
H6	0.2454	0.0945	−0.1602	0.059*
C7	0.14798 (13)	0.07811 (13)	0.0206 (3)	0.0482 (6)
C8	0.20198 (14)	0.03024 (15)	0.1632 (3)	0.0517 (6)
C9	0.30348 (13)	0.03373 (13)	0.1803 (3)	0.0420 (5)
C10	0.35019 (13)	0.10607 (14)	0.1603 (3)	0.0451 (5)
H10	0.3150	0.1511	0.1289	0.054*
C11	0.48557 (12)	0.04804 (12)	0.2241 (2)	0.0358 (5)
C12	0.44789 (12)	−0.02748 (12)	0.2511 (2)	0.0364 (5)
C13	0.35323 (13)	−0.03413 (13)	0.2305 (3)	0.0426 (5)
H13	0.3245	−0.0826	0.2500	0.051*
C14	0.52392 (13)	−0.07907 (13)	0.2957 (3)	0.0409 (5)
C15	0.52419 (16)	−0.16642 (14)	0.3369 (3)	0.0585 (6)
H15A	0.5858	−0.1858	0.3471	0.088*
H15B	0.4895	−0.1940	0.2360	0.088*
H15C	0.4975	−0.1757	0.4542	0.088*
C16	0.64979 (12)	0.09625 (12)	0.2357 (2)	0.0376 (5)
C17	0.73654 (13)	0.07915 (14)	0.3181 (3)	0.0484 (6)
H17	0.7475	0.0326	0.3881	0.058*
C18	0.80646 (14)	0.13251 (17)	0.2945 (3)	0.0618 (7)
H18	0.8650	0.1211	0.3478	0.074*
C19	0.79085 (16)	0.20215 (17)	0.1933 (3)	0.0639 (7)
H19	0.8384	0.2375	0.1783	0.077*
C20	0.70447 (15)	0.21893 (15)	0.1146 (3)	0.0548 (6)
H20	0.6935	0.2662	0.0473	0.066*
C21	0.63382 (14)	0.16638 (13)	0.1345 (3)	0.0448 (5)
H21	0.5756	0.1780	0.0800	0.054*
N1	0.44001 (10)	0.11614 (10)	0.1820 (2)	0.0426 (4)
N2	0.57850 (10)	0.03981 (10)	0.2511 (2)	0.0378 (4)
N3	0.60079 (11)	−0.03890 (10)	0.2955 (2)	0.0421 (4)
O1	0.01363 (10)	0.06702 (12)	0.1927 (3)	0.0870 (6)
H1	0.0497	0.0411	0.2629	0.130*
O2	0.16431 (10)	−0.01281 (12)	0.2757 (2)	0.0770 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0363 (13)	0.0691 (19)	0.0801 (16)	−0.0013 (12)	0.0012 (12)	−0.0142 (14)
C2	0.0360 (13)	0.078 (2)	0.108 (2)	0.0116 (13)	−0.0070 (14)	−0.0114 (17)
C3	0.0540 (16)	0.0674 (19)	0.0910 (19)	0.0122 (14)	−0.0217 (14)	−0.0046 (16)
C4	0.0514 (14)	0.0499 (16)	0.0636 (14)	0.0071 (12)	−0.0111 (11)	−0.0101 (12)
C5	0.0879 (19)	0.076 (2)	0.0695 (16)	0.0080 (16)	−0.0083 (14)	0.0057 (14)

C6	0.0362 (11)	0.0506 (15)	0.0591 (13)	0.0039 (10)	−0.0035 (10)	−0.0120 (11)
C7	0.0296 (11)	0.0521 (15)	0.0622 (13)	0.0028 (10)	−0.0007 (10)	−0.0120 (11)
C8	0.0384 (12)	0.0626 (17)	0.0542 (13)	−0.0040 (11)	0.0044 (10)	−0.0059 (12)
C9	0.0336 (11)	0.0484 (14)	0.0438 (11)	0.0006 (10)	0.0012 (8)	−0.0025 (10)
C10	0.0368 (12)	0.0459 (14)	0.0516 (12)	0.0073 (10)	−0.0020 (9)	−0.0009 (10)
C11	0.0317 (10)	0.0394 (13)	0.0361 (10)	0.0031 (9)	0.0016 (8)	−0.0025 (9)
C12	0.0366 (11)	0.0377 (13)	0.0348 (9)	0.0001 (9)	0.0025 (8)	−0.0048 (9)
C13	0.0425 (12)	0.0451 (14)	0.0407 (10)	−0.0082 (10)	0.0062 (9)	−0.0048 (9)
C14	0.0447 (12)	0.0382 (13)	0.0396 (10)	0.0015 (10)	0.0030 (9)	−0.0029 (9)
C15	0.0648 (15)	0.0400 (15)	0.0693 (14)	0.0025 (12)	−0.0020 (12)	0.0037 (11)
C16	0.0337 (11)	0.0435 (14)	0.0363 (10)	−0.0009 (9)	0.0071 (8)	−0.0068 (9)
C17	0.0373 (12)	0.0518 (15)	0.0558 (12)	0.0066 (11)	0.0023 (9)	−0.0054 (11)
C18	0.0319 (12)	0.076 (2)	0.0775 (16)	−0.0011 (12)	0.0064 (11)	−0.0127 (15)
C19	0.0485 (15)	0.072 (2)	0.0747 (16)	−0.0190 (13)	0.0219 (12)	−0.0100 (14)
C20	0.0579 (15)	0.0539 (16)	0.0541 (12)	−0.0116 (12)	0.0134 (11)	0.0017 (11)
C21	0.0432 (12)	0.0477 (15)	0.0432 (11)	−0.0032 (10)	0.0026 (9)	0.0001 (10)
N1	0.0340 (9)	0.0412 (11)	0.0520 (10)	0.0031 (8)	0.0003 (7)	−0.0012 (8)
N2	0.0324 (9)	0.0364 (11)	0.0443 (9)	0.0032 (8)	0.0013 (7)	0.0005 (8)
N3	0.0403 (10)	0.0367 (11)	0.0490 (9)	0.0066 (8)	0.0020 (7)	0.0006 (8)
O1	0.0393 (10)	0.1199 (18)	0.1043 (14)	−0.0003 (10)	0.0207 (9)	0.0018 (12)
O2	0.0431 (9)	0.1069 (16)	0.0816 (11)	−0.0112 (10)	0.0087 (8)	0.0238 (11)

Geometric parameters (Å, º)

C1—O1	1.349 (3)	C11—C12	1.399 (3)
C1—C2	1.391 (3)	C12—C13	1.393 (3)
C1—C7	1.403 (3)	C12—C14	1.427 (3)
C2—C3	1.372 (4)	C13—H13	0.9300
C2—H2	0.9300	C14—N3	1.316 (2)
C3—C4	1.390 (3)	C14—C15	1.490 (3)
C3—H3	0.9300	C15—H15A	0.9600
C4—C6	1.379 (3)	C15—H15B	0.9600
C4—C5	1.504 (3)	C15—H15C	0.9600
C5—H5A	0.9600	C16—C21	1.384 (3)
C5—H5B	0.9600	C16—C17	1.388 (3)
C5—H5C	0.9600	C16—N2	1.423 (2)
C6—C7	1.401 (3)	C17—C18	1.383 (3)
C6—H6	0.9300	C17—H17	0.9300
C7—C8	1.468 (3)	C18—C19	1.376 (3)
C8—O2	1.239 (3)	C18—H18	0.9300
C8—C9	1.489 (3)	C19—C20	1.373 (3)
C9—C13	1.381 (3)	C19—H19	0.9300
C9—C10	1.405 (3)	C20—C21	1.378 (3)
C10—N1	1.328 (2)	C20—H20	0.9300
C10—H10	0.9300	C21—H21	0.9300
C11—N1	1.343 (2)	N2—N3	1.387 (2)
C11—N2	1.372 (2)	O1—H1	0.8200

O1—C1—C2	118.1 (2)	C11—C12—C14	105.31 (17)
O1—C1—C7	122.7 (2)	C9—C13—C12	117.71 (19)
C2—C1—C7	119.2 (2)	C9—C13—H13	121.1
C3—C2—C1	120.5 (2)	C12—C13—H13	121.1
C3—C2—H2	119.8	N3—C14—C12	110.41 (18)
C1—C2—H2	119.8	N3—C14—C15	120.87 (19)
C2—C3—C4	122.0 (2)	C12—C14—C15	128.72 (19)
C2—C3—H3	119.0	C14—C15—H15A	109.5
C4—C3—H3	119.0	C14—C15—H15B	109.5
C6—C4—C3	117.3 (2)	H15A—C15—H15B	109.5
C6—C4—C5	121.2 (2)	C14—C15—H15C	109.5
C3—C4—C5	121.5 (2)	H15A—C15—H15C	109.5
C4—C5—H5A	109.5	H15B—C15—H15C	109.5
C4—C5—H5B	109.5	C21—C16—C17	120.13 (19)
H5A—C5—H5B	109.5	C21—C16—N2	120.56 (16)
C4—C5—H5C	109.5	C17—C16—N2	119.28 (18)
H5A—C5—H5C	109.5	C18—C17—C16	118.9 (2)
H5B—C5—H5C	109.5	C18—C17—H17	120.5
C4—C6—C7	122.6 (2)	C16—C17—H17	120.5
C4—C6—H6	118.7	C19—C18—C17	121.1 (2)
C7—C6—H6	118.7	C19—C18—H18	119.5
C6—C7—C1	118.5 (2)	C17—C18—H18	119.5
C6—C7—C8	121.67 (18)	C20—C19—C18	119.5 (2)
C1—C7—C8	119.8 (2)	C20—C19—H19	120.3
O2—C8—C7	120.86 (19)	C18—C19—H19	120.3
O2—C8—C9	118.09 (19)	C19—C20—C21	120.6 (2)
C7—C8—C9	121.03 (19)	C19—C20—H20	119.7
C13—C9—C10	118.74 (18)	C21—C20—H20	119.7
C13—C9—C8	119.7 (2)	C20—C21—C16	119.81 (19)
C10—C9—C8	121.43 (19)	C20—C21—H21	120.1
N1—C10—C9	126.03 (19)	C16—C21—H21	120.1
N1—C10—H10	117.0	C10—N1—C11	113.03 (18)
C9—C10—H10	117.0	C11—N2—N3	109.93 (16)
N1—C11—N2	126.11 (18)	C11—N2—C16	130.97 (17)
N1—C11—C12	126.89 (17)	N3—N2—C16	119.08 (15)
N2—C11—C12	107.00 (17)	C14—N3—N2	107.36 (15)
C13—C12—C11	117.53 (18)	C1—O1—H1	109.5
C13—C12—C14	137.2 (2)		

O1—C1—C2—C3	−177.8 (2)	C11—C12—C13—C9	1.6 (2)
C7—C1—C2—C3	2.0 (4)	C14—C12—C13—C9	−178.63 (19)
C1—C2—C3—C4	−0.3 (4)	C13—C12—C14—N3	−179.9 (2)
C2—C3—C4—C6	−0.9 (4)	C11—C12—C14—N3	−0.1 (2)
C2—C3—C4—C5	179.7 (2)	C13—C12—C14—C15	0.7 (4)
C3—C4—C6—C7	0.3 (3)	C11—C12—C14—C15	−179.57 (19)
C5—C4—C6—C7	179.8 (2)	C21—C16—C17—C18	−1.1 (3)
C4—C6—C7—C1	1.3 (3)	N2—C16—C17—C18	176.83 (17)
C4—C6—C7—C8	178.3 (2)	C16—C17—C18—C19	0.9 (3)

O1—C1—C7—C6	177.3 (2)	C17—C18—C19—C20	0.0 (4)
C2—C1—C7—C6	−2.4 (3)	C18—C19—C20—C21	−0.7 (3)
O1—C1—C7—C8	0.3 (4)	C19—C20—C21—C16	0.4 (3)
C2—C1—C7—C8	−179.5 (2)	C17—C16—C21—C20	0.5 (3)
C6—C7—C8—O2	−158.7 (2)	N2—C16—C21—C20	−177.45 (17)
C1—C7—C8—O2	18.2 (3)	C9—C10—N1—C11	1.0 (3)
C6—C7—C8—C9	23.0 (3)	N2—C11—N1—C10	178.78 (16)
C1—C7—C8—C9	−160.0 (2)	C12—C11—N1—C10	−2.1 (3)
O2—C8—C9—C13	36.0 (3)	N1—C11—N2—N3	178.98 (17)
C7—C8—C9—C13	−145.7 (2)	C12—C11—N2—N3	−0.31 (19)
O2—C8—C9—C10	−139.2 (2)	N1—C11—N2—C16	−2.9 (3)
C7—C8—C9—C10	39.1 (3)	C12—C11—N2—C16	177.79 (16)
C13—C9—C10—N1	1.3 (3)	C21—C16—N2—C11	−19.2 (3)
C8—C9—C10—N1	176.53 (18)	C17—C16—N2—C11	162.90 (18)
N1—C11—C12—C13	0.8 (3)	C21—C16—N2—N3	158.80 (17)
N2—C11—C12—C13	−179.92 (15)	C17—C16—N2—N3	−19.1 (2)
N1—C11—C12—C14	−179.01 (17)	C12—C14—N3—N2	0.0 (2)
N2—C11—C12—C14	0.27 (19)	C15—C14—N3—N2	179.44 (17)
C10—C9—C13—C12	−2.6 (3)	C11—N2—N3—C14	0.23 (19)
C8—C9—C13—C12	−177.90 (16)	C16—N2—N3—C14	−178.13 (14)

Hydrogen-bond geometry (Å, º)

Cg3 and Cg4 are the centroids of rings C1–C4/C6/C7 and C16–C21, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2	0.82	1.91	2.613 (2)	143
C21—H21···N1	0.93	2.41	3.019 (3)	123
C5—H5*A*···*Cg*3^{i}	0.96	2.97	3.703 (3)	134
C20—H20···*Cg*4^{i}	0.93	2.80	3.608 (2)	146

Symmetry code: (i) *x*, −*y*+1/2, *z*−1/2.