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3-Isopropyl-2-(4-methoxyphenoxy)-1-benzofuro[3,2-*d*]pyrimidin-4(3*H*)-one

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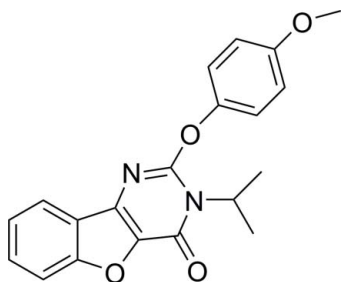
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 Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.070; wR factor = 0.155; data-to-parameter ratio = 16.0.

In the title compound, $\text{C}_{20}\text{H}_{18}\text{N}_2\text{O}_4$, all non-H atoms of the three fused rings of the benzofuro[3,2-*d*]pyrimidine system are almost coplanar (r.m.s. deviation 0.021 Å). The dihedral angle between the fused ring system and the benzene ring is $1.47(12)^\circ$. Intramolecular and intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds together with weak $\text{C}-\text{H}\cdots\pi$ interactions stabilize the structure.

Related literature

For the biological activity of benzofuro[3,2-*d*]pyrimidine derivatives, see: Bodke & Sangapure (2003). For the synthesis of the title compound, see: Ding *et al.* (2004). For the structures of other fused pyrimidinone derivatives, see: Hu *et al.* (2005, 2006, 2007).



Experimental

Crystal data

 $\text{C}_{20}\text{H}_{18}\text{N}_2\text{O}_4$
 $M_r = 350.36$

 Monoclinic, $P2_1/c$
 $a = 10.0358(7)$ Å
 $b = 14.2879(10)$ Å
 $c = 13.2071(9)$ Å
 $\beta = 112.089(1)^\circ$
 $V = 1754.8(2)$ Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.09$ mm⁻¹
 $T = 298$ K
 $0.26 \times 0.13 \times 0.10$ mm

Data collection

 Bruker SMART CCD area-detector diffractometer
 Absorption correction: none
 11156 measured reflections

 3809 independent reflections
 3354 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.040$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.070$
 $wR(F^2) = 0.155$
 $S = 1.22$
 3809 reflections

 238 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.19$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.23$ e Å⁻³

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C4}-\text{H4}\cdots\text{O4}^i$	0.93	2.49	3.311 (3)	147
$\text{C11}-\text{H11}\cdots\text{O2}$	0.98	2.25	2.761 (3)	111
$\text{C12}-\text{H12C}\cdots\text{O3}$	0.96	2.32	2.845 (4)	114
$\text{C13}-\text{H13A}\cdots\text{O3}$	0.96	2.41	2.957 (3)	116
$\text{C16}-\text{H16}\cdots\text{Cg2}^{ii}$	0.93	2.76	3.551 (2)	143
$\text{C19}-\text{H19}\cdots\text{Cg3}^{iii}$	0.93	2.90	3.742 (3)	152

Symmetry codes: (i) $-x + 2, -y + 1, -z$; (ii) $x, -y - \frac{1}{2}, z - \frac{3}{2}$; (iii) $-x + 2, y - \frac{1}{2}, -z + \frac{1}{2}$. Cg2 and Cg3 are the centroids of the $\text{N1/C8/C7/C10/N2/C9}$ and $\text{C1}-\text{C6}$ rings, respectively.

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: PLATON (Spek, 2009); software used to prepare material for publication: SHELXTL (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5104).

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supporting information

Acta Cryst. (2009). E65, o2839 [https://doi.org/10.1107/S1600536809042925]

3-Isopropyl-2-(4-methoxyphenoxy)-1-benzofuro[3,2-*d*]pyrimidin-4(3*H*)-one

Xiao-Bao Chen, Jing Xu, Ai-Hua Zheng, Jia-Hua Tian and Hong Luo

S1. Comment

Benzofuopyrimidine derivatives are of interest as possible antiviral agents, and because of their other biological properties, including antibacterial, antifungal, antiallergic and antiinflammatory activities (Bodke & Sangapure, 2003). We have recently focused on the synthesis of the fused heterocyclic systems containing pyrimidinone *via* aza-Wittig reactions at room temperature (Ding *et al.*, 2004). We present here the structure of such a benzofuopyrimidinone derivative. Fig. 1 shows the molecular structure of the title compound with the atomic numbering scheme. Intramolecular C—H \cdots O and intermolecular C—H \cdots O hydrogen bonds together with weak C—H \cdots π interactions (Table 1) stabilize the structure. (Fig.2).

S2. Experimental

To a solution of *N*-(2-ethoxycarbonylbenzofuran-3-yl)iminotriphenylphosphorane (3 mmol) in dry dichloromethane (15 ml) was added isopropyl isocyanate (3 mmol) under nitrogen at room temperature. After the reaction mixture had been allowed to stand for 20 h at 273–278 K, the solvent was removed under reduced pressure and diethyl ether-petroleum ether (1:2 *v/v*, 20 ml) was added to precipitate the triphenylphosphine oxide. After filtration, the solvent was removed to give the ethyl 3-((isopropylimino)methyleneamino)-2,3-dihydrobenzofuran-2-carboxylate, which was used directly without further purification. To a solution of ethyl 3-((isopropylimino)methyleneamino)-2,3-dihydrobenzofuran-2-carboxylate in acetonitrile (15 ml) were added 4-methylphenol (3 mmol) and anhydrous K₂CO₃ (1 mmol). The mixture was stirred for 6 h at 313–323 K. The solution was concentrated under reduced pressure and the residue was recrystallized from dichloromethane and ethanol (1:2 *v/v*) to give the title compound. Suitable crystals were obtained by vapour diffusion of ethanol into dichloromethane at room temperature.

S3. Refinement

H atoms were placed at calculated positions, with C—H distances of 0.97 and 0.93 Å for H atoms bonded to *sp*³ and *sp*² C atoms, respectively. They were refined using a riding model, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{methyl C})$.

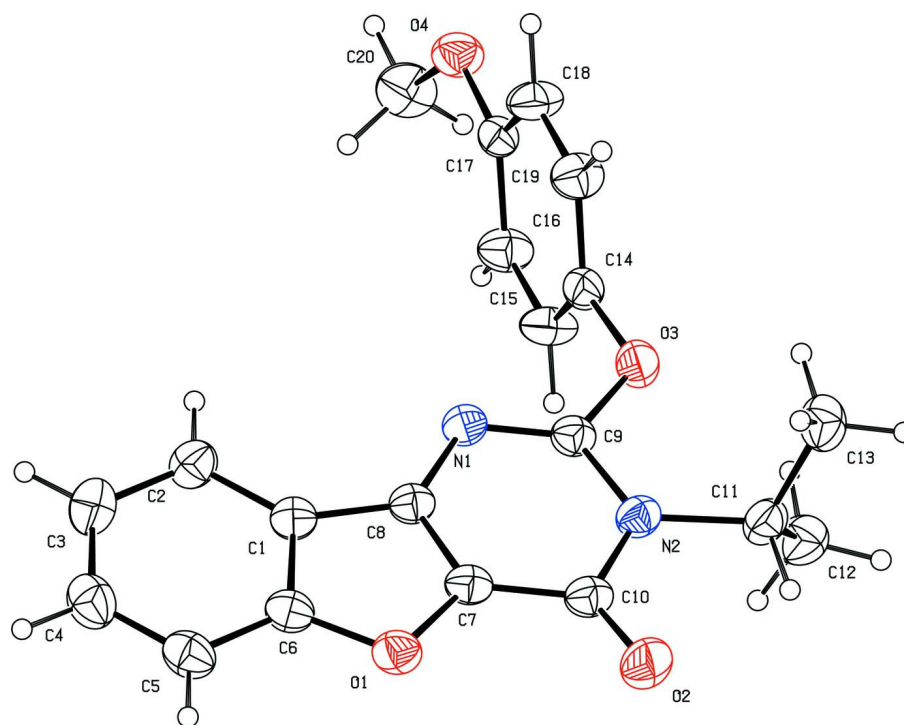


Figure 1

View of the molecular structure of (I), showing the atom labelling scheme and with displacement ellipsoids drawn at the 50% probability level.

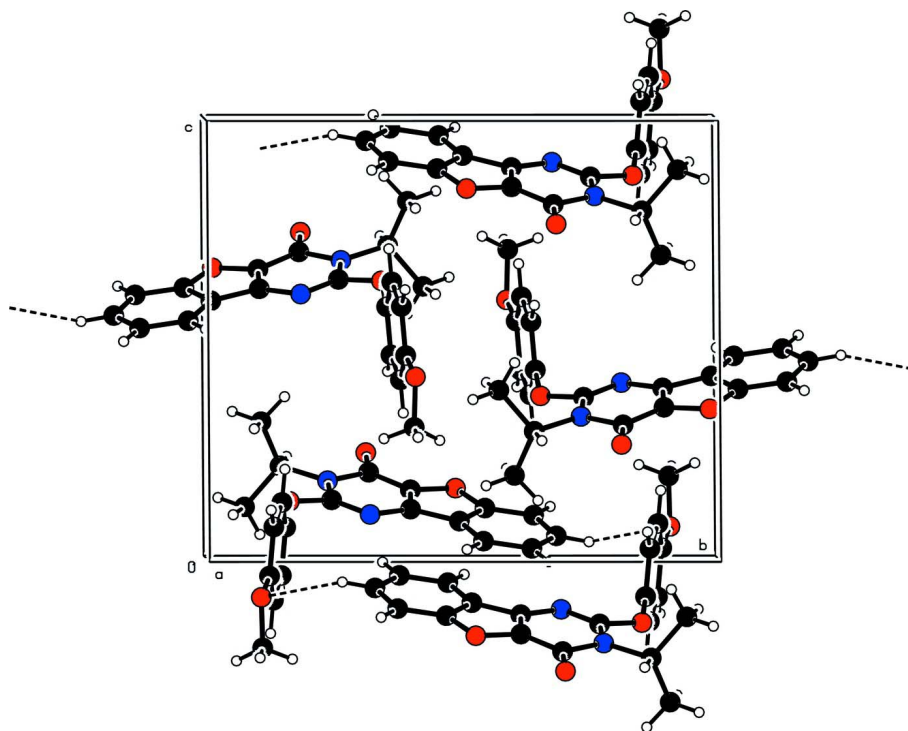


Figure 2

A partial view of the crystal packing of (I), showing the formation of C—H...O hydrogen-bonded. showing as dashed lines.

3-Isopropyl-2-(4-methoxyphenoxy)-1-benzofuro[3,2-*d*]pyrimidin- 4(3*H*)-one

Crystal data

$C_{20}H_{18}N_2O_4$

$M_r = 350.36$

Monoclinic, $P2_1/c$

$a = 10.0358 (7) \text{ \AA}$

$b = 14.2879 (10) \text{ \AA}$

$c = 13.2071 (9) \text{ \AA}$

$\beta = 112.089 (1)^\circ$

$V = 1754.8 (2) \text{ \AA}^3$

$Z = 4$

$F(000) = 736$

$D_x = 1.326 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 4035 reflections

$\theta = 2.2\text{--}27.2^\circ$

$\mu = 0.09 \text{ mm}^{-1}$

$T = 298 \text{ K}$

Block, colorless

$0.26 \times 0.13 \times 0.10 \text{ mm}$

Data collection

Bruker SMART CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

phi and ω scans

11156 measured reflections

3809 independent reflections

3354 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.040$

$\theta_{\text{max}} = 27.0^\circ$, $\theta_{\text{min}} = 2.2^\circ$

$h = -12 \rightarrow 12$

$k = -14 \rightarrow 18$

$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.070$
 $wR(F^2) = 0.155$
 $S = 1.22$
 3809 reflections
 238 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
 $w = 1/[\sigma^2(F_o^2) + (0.0482P)^2 + 0.6117P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.19 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.23 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.7439 (2)	0.49152 (15)	0.08888 (16)	0.0449 (5)
C2	0.8316 (3)	0.53714 (18)	0.04468 (19)	0.0556 (6)
H2	0.8998	0.5043	0.0268	0.067*
C3	0.8149 (3)	0.63207 (19)	0.0280 (2)	0.0665 (7)
H3	0.8725	0.6640	-0.0016	0.080*
C4	0.7126 (3)	0.68112 (18)	0.0549 (2)	0.0649 (7)
H4	0.7023	0.7451	0.0413	0.078*
C5	0.6270 (3)	0.63811 (17)	0.1005 (2)	0.0588 (6)
H5	0.5600	0.6713	0.1194	0.071*
C6	0.6450 (2)	0.54273 (16)	0.11700 (17)	0.0484 (5)
C7	0.6210 (2)	0.39759 (16)	0.15826 (17)	0.0453 (5)
C8	0.7248 (2)	0.39635 (15)	0.11576 (16)	0.0428 (5)
C9	0.7502 (2)	0.24186 (15)	0.13723 (17)	0.0440 (5)
C10	0.5734 (2)	0.31676 (17)	0.19732 (17)	0.0480 (5)
C11	0.6003 (2)	0.14330 (17)	0.21223 (19)	0.0523 (6)
H11	0.5180	0.1570	0.2325	0.063*
C12	0.5457 (3)	0.0739 (2)	0.1184 (2)	0.0671 (7)
H12A	0.4782	0.1044	0.0552	0.101*
H12B	0.4994	0.0226	0.1389	0.101*
H12C	0.6251	0.0508	0.1019	0.101*
C13	0.7157 (3)	0.10533 (19)	0.3141 (2)	0.0654 (7)
H13A	0.8000	0.0910	0.2992	0.098*
H13B	0.6815	0.0495	0.3369	0.098*
H13C	0.7390	0.1513	0.3712	0.098*
C14	0.9024 (2)	0.14978 (15)	0.07749 (18)	0.0448 (5)

C15	0.8475 (2)	0.14131 (19)	-0.0328 (2)	0.0605 (6)
H15	0.7490	0.1470	-0.0714	0.073*
C16	0.9378 (2)	0.12422 (18)	-0.08780 (19)	0.0567 (6)
H16	0.9002	0.1187	-0.1635	0.068*
C17	1.0832 (2)	0.11536 (14)	-0.03082 (18)	0.0438 (5)
C18	1.1364 (2)	0.12380 (19)	0.08137 (19)	0.0601 (6)
H18	1.2347	0.1177	0.1207	0.072*
C19	1.0466 (2)	0.14111 (19)	0.13570 (19)	0.0574 (6)
H19	1.0834	0.1469	0.2114	0.069*
C20	1.1334 (3)	0.1004 (2)	-0.1929 (2)	0.0735 (8)
H20A	1.0674	0.0498	-0.2234	0.110*
H20B	1.2143	0.0941	-0.2144	0.110*
H20C	1.0859	0.1589	-0.2192	0.110*
N1	0.79382 (18)	0.31642 (13)	0.10474 (14)	0.0452 (4)
N2	0.64378 (18)	0.23540 (13)	0.17913 (14)	0.0456 (4)
O1	0.56950 (16)	0.48638 (11)	0.16127 (13)	0.0528 (4)
O2	0.48616 (19)	0.31249 (13)	0.24071 (16)	0.0677 (5)
O3	0.80979 (17)	0.15842 (11)	0.13495 (14)	0.0561 (4)
O4	1.18117 (17)	0.09783 (12)	-0.07769 (13)	0.0584 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0430 (11)	0.0496 (12)	0.0382 (11)	-0.0016 (9)	0.0107 (9)	-0.0053 (9)
C2	0.0547 (13)	0.0561 (15)	0.0600 (14)	-0.0039 (11)	0.0262 (11)	-0.0047 (11)
C3	0.0730 (17)	0.0602 (16)	0.0691 (17)	-0.0135 (13)	0.0298 (14)	-0.0014 (13)
C4	0.0740 (17)	0.0493 (14)	0.0637 (16)	-0.0016 (12)	0.0171 (13)	-0.0009 (12)
C5	0.0604 (14)	0.0517 (14)	0.0591 (15)	0.0087 (11)	0.0165 (12)	-0.0055 (11)
C6	0.0458 (11)	0.0535 (13)	0.0413 (11)	0.0041 (10)	0.0112 (9)	-0.0028 (9)
C7	0.0404 (11)	0.0526 (13)	0.0428 (11)	0.0062 (9)	0.0154 (9)	-0.0020 (9)
C8	0.0387 (10)	0.0508 (12)	0.0369 (10)	0.0011 (9)	0.0121 (8)	-0.0028 (9)
C9	0.0417 (11)	0.0494 (12)	0.0416 (11)	0.0044 (9)	0.0165 (9)	0.0009 (9)
C10	0.0412 (11)	0.0598 (14)	0.0440 (12)	0.0039 (10)	0.0172 (9)	-0.0007 (10)
C11	0.0488 (12)	0.0560 (14)	0.0592 (14)	-0.0052 (10)	0.0283 (11)	0.0011 (11)
C12	0.0556 (14)	0.0657 (16)	0.0727 (17)	-0.0083 (12)	0.0159 (13)	-0.0067 (13)
C13	0.0754 (17)	0.0685 (17)	0.0530 (14)	-0.0054 (13)	0.0250 (13)	0.0105 (12)
C14	0.0465 (11)	0.0387 (11)	0.0533 (13)	0.0051 (9)	0.0236 (10)	0.0039 (9)
C15	0.0395 (11)	0.0805 (18)	0.0561 (15)	0.0139 (11)	0.0118 (10)	0.0019 (12)
C16	0.0485 (12)	0.0753 (17)	0.0423 (12)	0.0080 (11)	0.0126 (10)	-0.0022 (11)
C17	0.0438 (11)	0.0368 (11)	0.0532 (12)	0.0047 (8)	0.0210 (9)	0.0034 (9)
C18	0.0355 (11)	0.0880 (19)	0.0519 (14)	0.0053 (11)	0.0109 (10)	0.0042 (12)
C19	0.0516 (13)	0.0754 (17)	0.0435 (12)	0.0023 (12)	0.0158 (10)	0.0002 (11)
C20	0.0799 (18)	0.088 (2)	0.0628 (17)	0.0156 (15)	0.0391 (15)	-0.0024 (14)
N1	0.0425 (9)	0.0485 (10)	0.0489 (10)	0.0028 (8)	0.0220 (8)	-0.0005 (8)
N2	0.0415 (9)	0.0539 (11)	0.0432 (10)	-0.0009 (8)	0.0179 (8)	0.0001 (8)
O1	0.0511 (9)	0.0542 (9)	0.0589 (10)	0.0086 (7)	0.0272 (8)	-0.0022 (7)
O2	0.0671 (11)	0.0722 (12)	0.0841 (12)	0.0062 (9)	0.0517 (10)	0.0032 (9)
O3	0.0616 (10)	0.0494 (9)	0.0714 (11)	0.0106 (7)	0.0411 (8)	0.0114 (8)

O4	0.0529 (9)	0.0666 (11)	0.0617 (10)	0.0120 (8)	0.0285 (8)	0.0043 (8)
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Geometric parameters (Å, °)

C1—C2	1.388 (3)	C11—H11	0.9800
C1—C6	1.392 (3)	C12—H12A	0.9600
C1—C8	1.436 (3)	C12—H12B	0.9600
C2—C3	1.374 (4)	C12—H12C	0.9600
C2—H2	0.9300	C13—H13A	0.9600
C3—C4	1.395 (4)	C13—H13B	0.9600
C3—H3	0.9300	C13—H13C	0.9600
C4—C5	1.367 (4)	C14—C15	1.355 (3)
C4—H4	0.9300	C14—C19	1.365 (3)
C5—C6	1.381 (3)	C14—O3	1.409 (2)
C5—H5	0.9300	C15—C16	1.380 (3)
C6—O1	1.377 (3)	C15—H15	0.9300
C7—C8	1.357 (3)	C16—C17	1.373 (3)
C7—O1	1.376 (3)	C16—H16	0.9300
C7—C10	1.418 (3)	C17—O4	1.368 (2)
C8—N1	1.372 (3)	C17—C18	1.378 (3)
C9—N1	1.285 (3)	C18—C19	1.369 (3)
C9—O3	1.339 (3)	C18—H18	0.9300
C9—N2	1.378 (3)	C19—H19	0.9300
C10—O2	1.215 (3)	C20—O4	1.414 (3)
C10—N2	1.427 (3)	C20—H20A	0.9600
C11—N2	1.502 (3)	C20—H20B	0.9600
C11—C13	1.508 (3)	C20—H20C	0.9600
C11—C12	1.519 (3)		
C2—C1—C6	119.6 (2)	H12A—C12—H12C	109.5
C2—C1—C8	135.5 (2)	H12B—C12—H12C	109.5
C6—C1—C8	104.85 (19)	C11—C13—H13A	109.5
C3—C2—C1	118.2 (2)	C11—C13—H13B	109.5
C3—C2—H2	120.9	H13A—C13—H13B	109.5
C1—C2—H2	120.9	C11—C13—H13C	109.5
C2—C3—C4	120.8 (2)	H13A—C13—H13C	109.5
C2—C3—H3	119.6	H13B—C13—H13C	109.5
C4—C3—H3	119.6	C15—C14—C19	120.9 (2)
C5—C4—C3	122.1 (2)	C15—C14—O3	120.16 (19)
C5—C4—H4	119.0	C19—C14—O3	118.6 (2)
C3—C4—H4	119.0	C14—C15—C16	120.0 (2)
C4—C5—C6	116.5 (2)	C14—C15—H15	120.0
C4—C5—H5	121.7	C16—C15—H15	120.0
C6—C5—H5	121.7	C17—C16—C15	120.0 (2)
O1—C6—C5	125.7 (2)	C17—C16—H16	120.0
O1—C6—C1	111.57 (19)	C15—C16—H16	120.0
C5—C6—C1	122.7 (2)	O4—C17—C16	124.4 (2)
C8—C7—O1	112.26 (19)	O4—C17—C18	116.66 (19)

C8—C7—C10	123.7 (2)	C16—C17—C18	118.9 (2)
O1—C7—C10	123.99 (18)	C19—C18—C17	120.9 (2)
C7—C8—N1	123.5 (2)	C19—C18—H18	119.5
C7—C8—C1	106.56 (19)	C17—C18—H18	119.5
N1—C8—C1	129.93 (18)	C14—C19—C18	119.2 (2)
N1—C9—O3	121.27 (18)	C14—C19—H19	120.4
N1—C9—N2	127.03 (19)	C18—C19—H19	120.4
O3—C9—N2	111.69 (18)	O4—C20—H20A	109.5
O2—C10—C7	127.8 (2)	O4—C20—H20B	109.5
O2—C10—N2	121.9 (2)	H20A—C20—H20B	109.5
C7—C10—N2	110.30 (17)	O4—C20—H20C	109.5
N2—C11—C13	111.44 (18)	H20A—C20—H20C	109.5
N2—C11—C12	112.94 (19)	H20B—C20—H20C	109.5
C13—C11—C12	114.4 (2)	C9—N1—C8	113.92 (17)
N2—C11—H11	105.7	C9—N2—C10	121.34 (18)
C13—C11—H11	105.7	C9—N2—C11	121.94 (18)
C12—C11—H11	105.7	C10—N2—C11	116.67 (17)
C11—C12—H12A	109.5	C7—O1—C6	104.74 (16)
C11—C12—H12B	109.5	C9—O3—C14	118.74 (16)
H12A—C12—H12B	109.5	C17—O4—C20	118.16 (19)
C11—C12—H12C	109.5		
C6—C1—C2—C3	-1.4 (3)	C15—C14—C19—C18	0.1 (4)
C8—C1—C2—C3	178.1 (2)	O3—C14—C19—C18	173.9 (2)
C1—C2—C3—C4	0.0 (4)	C17—C18—C19—C14	0.2 (4)
C2—C3—C4—C5	1.3 (4)	O3—C9—N1—C8	-177.98 (18)
C3—C4—C5—C6	-1.1 (4)	N2—C9—N1—C8	0.8 (3)
C4—C5—C6—O1	-179.7 (2)	C7—C8—N1—C9	0.8 (3)
C4—C5—C6—C1	-0.3 (3)	C1—C8—N1—C9	179.9 (2)
C2—C1—C6—O1	-178.92 (19)	N1—C9—N2—C10	-3.9 (3)
C8—C1—C6—O1	1.4 (2)	O3—C9—N2—C10	174.94 (17)
C2—C1—C6—C5	1.6 (3)	N1—C9—N2—C11	178.7 (2)
C8—C1—C6—C5	-178.1 (2)	O3—C9—N2—C11	-2.5 (3)
O1—C7—C8—N1	179.51 (18)	O2—C10—N2—C9	-175.2 (2)
C10—C7—C8—N1	0.8 (3)	C7—C10—N2—C9	4.8 (3)
O1—C7—C8—C1	0.2 (2)	O2—C10—N2—C11	2.4 (3)
C10—C7—C8—C1	-178.48 (19)	C7—C10—N2—C11	-177.66 (17)
C2—C1—C8—C7	179.5 (2)	C13—C11—N2—C9	70.7 (3)
C6—C1—C8—C7	-1.0 (2)	C12—C11—N2—C9	-59.8 (3)
C2—C1—C8—N1	0.2 (4)	C13—C11—N2—C10	-106.9 (2)
C6—C1—C8—N1	179.8 (2)	C12—C11—N2—C10	122.7 (2)
C8—C7—C10—O2	176.5 (2)	C8—C7—O1—C6	0.7 (2)
O1—C7—C10—O2	-2.0 (4)	C10—C7—O1—C6	179.3 (2)
C8—C7—C10—N2	-3.5 (3)	C5—C6—O1—C7	178.2 (2)
O1—C7—C10—N2	177.99 (18)	C1—C6—O1—C7	-1.3 (2)
C19—C14—C15—C16	-0.4 (4)	N1—C9—O3—C14	-11.9 (3)
O3—C14—C15—C16	-174.0 (2)	N2—C9—O3—C14	169.19 (17)
C14—C15—C16—C17	0.3 (4)	C15—C14—O3—C9	-79.2 (3)

C15—C16—C17—O4	179.5 (2)	C19—C14—O3—C9	107.1 (2)
C15—C16—C17—C18	0.0 (4)	C16—C17—O4—C20	8.2 (3)
O4—C17—C18—C19	-179.8 (2)	C18—C17—O4—C20	-172.2 (2)
C16—C17—C18—C19	-0.3 (4)		

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>
C4—H4 \cdots O4 ⁱ	0.93	2.49	3.311 (3)	147
C11—H11 \cdots O2	0.98	2.25	2.761 (3)	111
C12—H12C \cdots O3	0.96	2.32	2.845 (4)	114
C13—H13A \cdots O3	0.96	2.41	2.957 (3)	116
C16—H16 \cdots Cg2 ⁱⁱ	0.93	2.76	3.551 (2)	143
C19—H19 \cdots Cg3 ⁱⁱⁱ	0.93	2.90	3.742 (3)	152

Symmetry codes: (i) $-x+2, -y+1, -z$; (ii) $x, -y-1/2, z-3/2$; (iii) $-x+2, y-1/2, -z+1/2$.