organic compounds

3-Benzyl-6-isopropyl-5-phenoxy-3*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7(6*H*)-one

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In the title compound, $C_{20}H_{19}N_5O_2$, all atoms of the 1,2,3-triazolo[4,5-*d*]pyrimidine ring system are essentially coplanar [maximum deviation = 0.015 (2) Å], indicating the existence of a conjugate system in which each carbon and nitrogen atom is sp^2 hybridized and ten π electrons (three from carbon atoms and seven from nitrogen atoms) constitute an aromatic heterocycle. The ring system forms dihedral angles of 68.37 (10) and 71.57 (9)° with the phenyl rings. The crystal packing is stabilized by van der Waals interactions and intermolecular C—H$\cdots\pi$ interactions.

Related literature

For the biological activity of 8-azaguanine derivatives, see: Roblin *et al.* (1945); Ding *et al.* (2004); Mitchell *et al.* (1950); Levine *et al.* (1963); Montgomery *et al.* (1962); Yamamoto *et al.* (1967); Bariana (1971); Holland *et al.* (1975). For related structures, see: Ferguson *et al.* (1998); Li *et al.* (2004); Zhao, Xie *et al.* (2005); Zhao, Hu *et al.* (2005); Zhao, Wang & Ding (2005); Chen & Shi (2006); Maldonado *et al.* (2006); Xiao & Shi (2007); Wang *et al.* (2006, 2008); Zeng, Deng, Qu & Wang (2009); Zeng, Deng, Chen *et al.* (2009); Zeng, Liu *et al.* (2009).
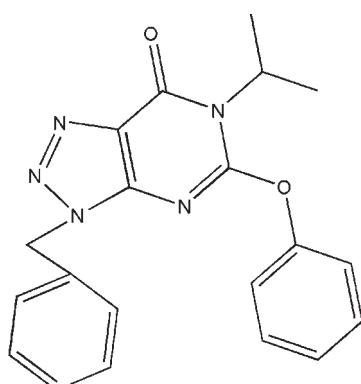
Experimental

Crystal data

$C_{20}H_{19}N_5O_2$	$V = 1858.0$ (4) Å^3
$M_r = 361.40$	$Z = 4$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 9.4585$ (13) Å	$\mu = 0.09$ mm^{-1}
$b = 9.0846$ (12) Å	$T = 298$ K
$c = 21.992$ (3) Å	$0.16 \times 0.13 \times 0.10$ mm
$\beta = 100.523$ (2)°	

Data collection

Bruker SMART CCD area-detector diffractometer	10907 measured reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	3655 independent reflections
	3079 reflections with $I > 2\sigma(I)$
$T_{min} = 0.986$, $T_{max} = 0.991$	$R_{int} = 0.074$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.067$	246 parameters
$wR(F^2) = 0.167$	H-atom parameters constrained
$S = 1.14$	$\Delta\rho_{max} = 0.19$ e Å^{-3}
3655 reflections	$\Delta\rho_{min} = -0.31$ e Å^{-3}

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C13—H13$A\cdots Cg^i$	0.96	2.75	3.696 (3)	171

Symmetry code: (i) $-x, y - \frac{1}{2}, -z + \frac{1}{2}$. Cg is the centroid of the C15–C20 phenyl ring.

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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supporting information

3-Benzyl-6-isopropyl-5-phenoxy-3*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7(6*H*)-one

Shou-Heng Deng, Hong-Mei Wang, Ping Chen, Jun-Kai Ma and Feng-Jun Cao

S1. Comment

The derivatives of heterocycles containing 8-azaguanine system, which are well known bioisosteres of guanine, are of great importance because of their remarkable biological properties. Some of these activities include antimicrobial or antifungal activities (Roblin *et al.*, 1945; Ding *et al.*, 2004), encephaloma cell inhibitor activity (Mitchell *et al.*, 1950; Levine *et al.*, 1963), antileukemie activity (Montgomery *et al.*, 1962), hypersusceptibility inhibitor activity and acesodyne activity (Yamamoto *et al.*, 1967; Bariana, 1971; Holland *et al.*, 1975).

In recent years, we have been engaged in the preparation of derivatives of 8-azaguanine *via* aza-Wittig reaction of beta-ethoxycarbonyl iminophosphorane with aromatic isocyanate (Zhao, Xie *et al.*, 2005). As a continuation of our research for new biologically active heterocycles, the title compound was obtained from beta-ethoxycarbonyl iminophosphorane with alphalic isocyanate, and structurally characterized in this context.

In the title compound (Fig. 1), bond lengths and angles within the triazolopyrimidinone moiety are in good agreement with those observed for closely related structures (Zhao, Hu *et al.*, 2005; Zhao, Wang & Ding, 2005). As reported for related compounds (Ferguson *et al.*, 1998; Maldonado *et al.*, 2006; Zeng, Deng, Qu *et al.*, 2009; Zeng, Deng, Chen *et al.*, 2009; Zeng, Liu *et al.*, 2009; Wang *et al.*, 2008; Xiao & Shi, 2007; Chen & Shi, 2007), all atoms in the 1,2,3-triazolo[4,5-*d*]pyrimidine ring system are essentially coplanar (maximum deviation 0.015 (2)Å for atom N2), indicating that the 1,2,3-triazolo[4,5-*d*]pyrimidine moiety is a conjugate system, in which each carbon and nitrogen atom is sp^2 hybridized and ten π electrons (three from carbon atoms and seven from nitrogen atoms) constitute an aromatic heterocycle (Li *et al.*, 2004). The dihedral angles it forms with the C4–C9 and C15–C20 phenyl rings are 68.37 (10) and 71.57 (9)°, respectively.

The crystal packing is stabilized mainly by van der Waals interactions, no intermolecular hydrogen bonds or π–π stacking interactions being observed. One of the methyl H atoms is involved in a contact to the centroid (Cg) of the C15/C20 phenyl ring (C13–H13A⋯Cg = 2.75 Å), which may be considered as a C—H⋯π interaction.

S2. Experimental

To a solution of carbodiimide in CH_2Cl_2/CH_3CN (1:4 *v*/*v*, 15 ml) prepared according to the literature method (Wang *et al.*, 2006), was added phenol (3 mmol) and excess K_2CO_3, and the reaction mixture was stirred for 12 h. The solvent was removed under reduced pressure and the residue was recrystallized from EtOH to give the title compound (yield 75%; m.p. 405 K). Elemental analysis: calculated for $C_{20}H_{19}N_5O_2$: C, 66.47; H, 5.30; N, 19.38%. Found: C, 65.67; H, 5.56; N, 18.92%. Crystals suitable for single-crystal X-ray diffraction analysis were obtained by slow evaporation of a hexane/dichloromethane (1:3 *v*/*v*) solution at room temperature.

S3. Refinement

H atoms were placed at calculated positions and treated as riding atoms, with C—H = 0.93–0.98 Å, and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C) for methyl H atoms.
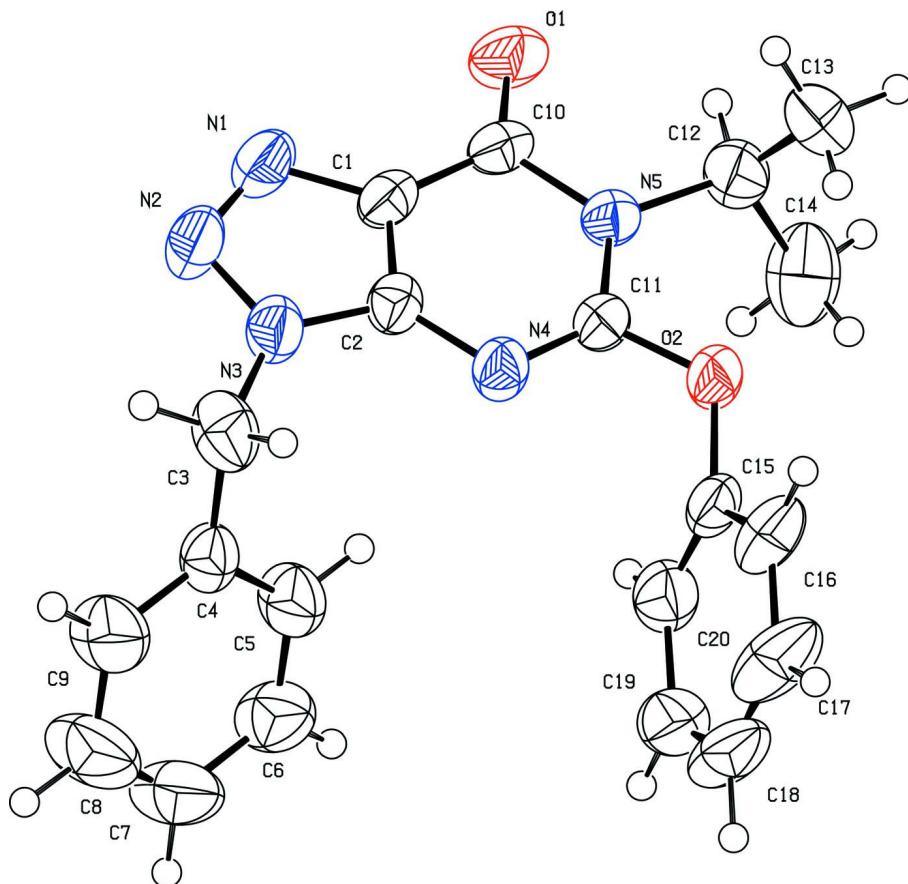
Figure 1

The molecular structure of the title compound showing the atom-labeling scheme. Displacement ellipsoids are drawn at 50% probability level. H-atoms are represented by circles of arbitrary size.

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Crystal data

$C_{20}H_{19}N_5O_2$	$F(000) = 760$
$M_r = 361.40$	$D_x = 1.292$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 3682 reflections
$a = 9.4585$ (13) Å	$\theta = 2.4–25.1°$
$b = 9.0846$ (12) Å	$\mu = 0.09$ mm^{-1}
$c = 21.992$ (3) Å	$T = 298$ K
$\beta = 100.523$ (2)°	Block, colourless
$V = 1858.0$ (4) Å^3	$0.16 \times 0.13 \times 0.10$ mm
$Z = 4$	

Data collection

Bruker SMART CCD area-detector diffractometer	Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
Radiation source: fine-focus sealed tube	$T_{min} = 0.986$, $T_{max} = 0.991$
Graphite monochromator	10907 measured reflections
φ and ω scans	3655 independent reflections
	3079 reflections with $I > 2\sigma(I)$

$R_{int} = 0.074$

$\theta_{max} = 26.0°, \theta_{min} = 1.9°$

$h = -8 \rightarrow 11$

$k = -11 \rightarrow 11$

$l = -27 \rightarrow 27$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.067$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.167$	
$S = 1.14$	H-atom parameters constrained
3655 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0685P)^2 + 0.418P]$
246 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	$\Delta\rho_{max} = 0.19$ e Å^{-3}
	$\Delta\rho_{min} = -0.31$ 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	0.3436 (2)	0.4731 (2)	0.22493 (9)	0.0422 (5)
C2	0.3377 (2)	0.4926 (2)	0.28596 (9)	0.0400 (5)
C3	0.4595 (3)	0.3594 (3)	0.38253 (11)	0.0615 (6)
H3A	0.4907	0.2579	0.3884	0.074*
H3B	0.3730	0.3701	0.4000	0.074*
C4	0.5747 (2)	0.4573 (2)	0.41799 (10)	0.0486 (5)
C5	0.5893 (3)	0.6038 (3)	0.40342 (11)	0.0616 (6)
H5	0.5277	0.6448	0.3699	0.074*
C6	0.6935 (3)	0.6893 (3)	0.43782 (12)	0.0697 (7)
H6	0.7016	0.7878	0.4276	0.084*
C7	0.7851 (4)	0.6317 (3)	0.48672 (12)	0.0810 (9)
H7	0.8549	0.6906	0.5103	0.097*
C8	0.7738 (4)	0.4858 (4)	0.50106 (13)	0.0974 (11)
H8	0.8373	0.4450	0.5340	0.117*
C9	0.6685 (3)	0.3994 (3)	0.46668 (12)	0.0751 (8)
H9	0.6614	0.3006	0.4768	0.090*
C10	0.2657 (2)	0.5691 (2)	0.17917 (9)	0.0435 (5)
C11	0.1931 (2)	0.6823 (2)	0.26940 (9)	0.0409 (5)
C12	0.0995 (3)	0.7849 (3)	0.16396 (10)	0.0594 (6)
H12	0.1186	0.7635	0.1225	0.071*
C13	−0.0597 (3)	0.7597 (3)	0.16099 (13)	0.0810 (9)
H13A	−0.0837	0.6606	0.1478	0.121*

H13B	−0.1133	0.8274	0.1321	0.121*
H13C	−0.0831	0.7751	0.2012	0.121*
C14	0.1452 (4)	0.9438 (3)	0.17780 (15)	0.0853 (9)
H14A	0.1002	0.9807	0.2105	0.128*
H14B	0.1163	1.0025	0.1414	0.128*
H14C	0.2478	0.9483	0.1903	0.128*
C15	0.1523 (3)	0.8427 (2)	0.34770 (9)	0.0479 (5)
C16	0.0476 (3)	0.8378 (3)	0.38311 (12)	0.0635 (7)
H16	−0.0422	0.7977	0.3677	0.076*
C17	0.0788 (4)	0.8938 (3)	0.44193 (13)	0.0838 (10)
H17	0.0090	0.8917	0.4667	0.101*
C18	0.2099 (4)	0.9524 (3)	0.46459 (11)	0.0810 (10)
H18	0.2297	0.9888	0.5048	0.097*
C19	0.3141 (3)	0.9579 (3)	0.42792 (12)	0.0723 (8)
H19	0.4035	0.9991	0.4432	0.087*
C20	0.2849 (3)	0.9021 (3)	0.36845 (10)	0.0591 (6)
H20	0.3538	0.9049	0.3432	0.071*
N1	0.4331 (2)	0.3583 (2)	0.21950 (10)	0.0601 (5)
N2	0.4819 (2)	0.3075 (2)	0.27476 (11)	0.0633 (6)
N3	0.42351 (19)	0.38878 (19)	0.31642 (8)	0.0488 (5)
N4	0.26237 (18)	0.59583 (19)	0.31105 (7)	0.0444 (4)
N5	0.18677 (18)	0.67677 (18)	0.20678 (7)	0.0411 (4)
O1	0.26306 (19)	0.56707 (19)	0.12390 (7)	0.0635 (5)
O2	0.11490 (17)	0.79269 (18)	0.28643 (6)	0.0572 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0411 (11)	0.0384 (10)	0.0493 (11)	−0.0012 (8)	0.0138 (9)	−0.0112 (8)
C2	0.0374 (10)	0.0343 (9)	0.0487 (11)	0.0003 (8)	0.0094 (9)	−0.0007 (8)
C3	0.0607 (15)	0.0502 (13)	0.0711 (16)	0.0003 (11)	0.0051 (12)	0.0202 (11)
C4	0.0540 (13)	0.0454 (11)	0.0475 (12)	0.0092 (10)	0.0123 (10)	0.0075 (9)
C5	0.0682 (16)	0.0488 (13)	0.0632 (15)	0.0028 (12)	0.0000 (12)	0.0114 (11)
C6	0.091 (2)	0.0526 (14)	0.0628 (16)	−0.0057 (14)	0.0072 (14)	0.0002 (11)
C7	0.106 (2)	0.0769 (19)	0.0526 (15)	−0.0154 (17)	−0.0042 (15)	−0.0061 (13)
C8	0.125 (3)	0.089 (2)	0.0612 (17)	−0.006 (2)	−0.0294 (18)	0.0158 (15)
C9	0.100 (2)	0.0570 (15)	0.0616 (15)	0.0009 (15)	−0.0032 (15)	0.0169 (12)
C10	0.0478 (12)	0.0438 (11)	0.0403 (11)	−0.0039 (9)	0.0115 (9)	−0.0117 (8)
C11	0.0415 (11)	0.0433 (11)	0.0387 (10)	0.0057 (9)	0.0089 (8)	−0.0045 (8)
C12	0.0767 (17)	0.0649 (15)	0.0354 (11)	0.0199 (13)	0.0073 (11)	0.0058 (10)
C13	0.0683 (18)	0.0792 (18)	0.0812 (19)	0.0162 (15)	−0.0237 (15)	−0.0102 (15)
C14	0.095 (2)	0.0628 (17)	0.103 (2)	0.0139 (16)	0.0296 (18)	0.0320 (16)
C15	0.0629 (14)	0.0431 (11)	0.0394 (11)	0.0186 (10)	0.0133 (10)	−0.0029 (8)
C16	0.0803 (18)	0.0497 (13)	0.0690 (15)	0.0098 (12)	0.0361 (14)	−0.0083 (11)
C17	0.137 (3)	0.0626 (17)	0.0659 (18)	0.0074 (19)	0.0572 (19)	−0.0088 (14)
C18	0.152 (3)	0.0538 (15)	0.0372 (12)	0.0233 (18)	0.0171 (17)	−0.0061 (11)
C19	0.093 (2)	0.0560 (15)	0.0598 (15)	0.0115 (14)	−0.0083 (14)	−0.0043 (12)
C20	0.0656 (16)	0.0636 (15)	0.0489 (13)	0.0154 (13)	0.0126 (11)	0.0025 (11)

N1	0.0563 (12)	0.0541 (11)	0.0707 (13)	0.0107 (9)	0.0138 (10)	−0.0194 (10)
N2	0.0584 (13)	0.0452 (11)	0.0843 (15)	0.0133 (9)	0.0081 (11)	−0.0134 (10)
N3	0.0466 (10)	0.0381 (9)	0.0604 (11)	0.0049 (8)	0.0063 (8)	0.0010 (8)
N4	0.0486 (10)	0.0474 (10)	0.0387 (9)	0.0117 (8)	0.0121 (7)	0.0014 (7)
N5	0.0456 (10)	0.0428 (9)	0.0350 (8)	0.0036 (7)	0.0079 (7)	−0.0024 (7)
O1	0.0826 (12)	0.0719 (11)	0.0383 (8)	0.0049 (9)	0.0172 (8)	−0.0126 (7)
O2	0.0638 (10)	0.0664 (10)	0.0401 (8)	0.0306 (8)	0.0057 (7)	−0.0096 (7)

Geometric parameters (Å, º)

C1—N1	1.362 (3)	C12—N5	1.500 (3)
C1—C2	1.365 (3)	C12—C13	1.513 (4)
C1—C10	1.430 (3)	C12—C14	1.521 (4)
C2—N3	1.341 (2)	C12—H12	0.9800
C2—N4	1.355 (2)	C13—H13A	0.9600
C3—N3	1.456 (3)	C13—H13B	0.9600
C3—C4	1.509 (3)	C13—H13C	0.9600
C3—H3A	0.9700	C14—H14A	0.9600
C3—H3B	0.9700	C14—H14B	0.9600
C4—C9	1.365 (3)	C14—H14C	0.9600
C4—C5	1.382 (3)	C15—C20	1.365 (3)
C5—C6	1.369 (3)	C15—C16	1.367 (3)
C5—H5	0.9300	C15—O2	1.405 (2)
C6—C7	1.356 (4)	C16—C17	1.371 (4)
C6—H6	0.9300	C16—H16	0.9300
C7—C8	1.371 (4)	C17—C18	1.358 (5)
C7—H7	0.9300	C17—H17	0.9300
C8—C9	1.380 (4)	C18—C19	1.383 (4)
C8—H8	0.9300	C18—H18	0.9300
C9—H9	0.9300	C19—C20	1.383 (3)
C10—O1	1.211 (2)	C19—H19	0.9300
C10—N5	1.431 (2)	C20—H20	0.9300
C11—N4	1.291 (2)	N1—N2	1.303 (3)
C11—O2	1.339 (2)	N2—N3	1.369 (3)
C11—N5	1.368 (2)		
N1—C1—C2	108.83 (19)	C14—C12—H12	106.3
N1—C1—C10	130.83 (19)	C12—C13—H13A	109.5
C2—C1—C10	120.31 (18)	C12—C13—H13B	109.5
N3—C2—N4	126.77 (18)	H13A—C13—H13B	109.5
N3—C2—C1	105.72 (17)	C12—C13—H13C	109.5
N4—C2—C1	127.51 (18)	H13A—C13—H13C	109.5
N3—C3—C4	115.02 (18)	H13B—C13—H13C	109.5
N3—C3—H3A	108.5	C12—C14—H14A	109.5
C4—C3—H3A	108.5	C12—C14—H14B	109.5
N3—C3—H3B	108.5	H14A—C14—H14B	109.5
C4—C3—H3B	108.5	C12—C14—H14C	109.5
H3A—C3—H3B	107.5	H14A—C14—H14C	109.5

C9—C4—C5	118.3 (2)	H14B—C14—H14C	109.5
C9—C4—C3	118.9 (2)	C20—C15—C16	122.6 (2)
C5—C4—C3	122.7 (2)	C20—C15—O2	120.2 (2)
C6—C5—C4	120.7 (2)	C16—C15—O2	117.0 (2)
C6—C5—H5	119.7	C15—C16—C17	118.2 (3)
C4—C5—H5	119.7	C15—C16—H16	120.9
C7—C6—C5	120.7 (2)	C17—C16—H16	120.9
C7—C6—H6	119.6	C18—C17—C16	121.1 (3)
C5—C6—H6	119.6	C18—C17—H17	119.5
C6—C7—C8	119.3 (3)	C16—C17—H17	119.5
C6—C7—H7	120.3	C17—C18—C19	120.0 (2)
C8—C7—H7	120.3	C17—C18—H18	120.0
C7—C8—C9	120.2 (3)	C19—C18—H18	120.0
C7—C8—H8	119.9	C20—C19—C18	119.8 (3)
C9—C8—H8	119.9	C20—C19—H19	120.1
C4—C9—C8	120.8 (2)	C18—C19—H19	120.1
C4—C9—H9	119.6	C15—C20—C19	118.3 (2)
C8—C9—H9	119.6	C15—C20—H20	120.9
O1—C10—C1	127.61 (19)	C19—C20—H20	120.9
O1—C10—N5	121.29 (19)	N2—N1—C1	108.03 (18)
C1—C10—N5	111.10 (16)	N1—N2—N3	108.40 (17)
N4—C11—O2	119.46 (17)	C2—N3—N2	109.02 (18)
N4—C11—N5	127.95 (18)	C2—N3—C3	129.62 (19)
O2—C11—N5	112.58 (16)	N2—N3—C3	121.34 (19)
N5—C12—C13	110.9 (2)	C11—N4—C2	111.65 (16)
N5—C12—C14	113.1 (2)	C11—N5—C10	121.45 (16)
C13—C12—C14	113.3 (2)	C11—N5—C12	121.72 (16)
N5—C12—H12	106.3	C10—N5—C12	116.81 (16)
C13—C12—H12	106.3	C11—O2—C15	117.06 (15)
N1—C1—C2—N3	−0.2 (2)	N4—C2—N3—N2	−179.02 (19)
C10—C1—C2—N3	−178.61 (18)	C1—C2—N3—N2	0.4 (2)
N1—C1—C2—N4	179.23 (19)	N4—C2—N3—C3	−0.5 (3)
C10—C1—C2—N4	0.8 (3)	C1—C2—N3—C3	178.9 (2)
N3—C3—C4—C9	−145.0 (2)	N1—N2—N3—C2	−0.5 (2)
N3—C3—C4—C5	35.3 (3)	N1—N2—N3—C3	−179.14 (19)
C9—C4—C5—C6	−1.3 (4)	C4—C3—N3—C2	−80.8 (3)
C3—C4—C5—C6	178.5 (2)	C4—C3—N3—N2	97.6 (2)
C4—C5—C6—C7	0.3 (4)	O2—C11—N4—C2	−178.81 (18)
C5—C6—C7—C8	0.9 (5)	N5—C11—N4—C2	1.8 (3)
C6—C7—C8—C9	−1.2 (6)	N3—C2—N4—C11	178.18 (19)
C5—C4—C9—C8	1.0 (4)	C1—C2—N4—C11	−1.1 (3)
C3—C4—C9—C8	−178.8 (3)	N4—C11—N5—C10	−2.1 (3)
C7—C8—C9—C4	0.2 (5)	O2—C11—N5—C10	178.45 (17)
N1—C1—C10—O1	0.3 (4)	N4—C11—N5—C12	179.2 (2)
C2—C1—C10—O1	178.4 (2)	O2—C11—N5—C12	−0.2 (3)
N1—C1—C10—N5	−178.9 (2)	O1—C10—N5—C11	−177.88 (19)
C2—C1—C10—N5	−0.8 (3)	C1—C10—N5—C11	1.4 (3)

C20—C15—C16—C17	−0.7 (4)	O1—C10—N5—C12	0.9 (3)
O2—C15—C16—C17	−176.3 (2)	C1—C10—N5—C12	−179.87 (18)
C15—C16—C17—C18	−0.1 (4)	C13—C12—N5—C11	−69.5 (3)
C16—C17—C18—C19	0.8 (4)	C14—C12—N5—C11	59.1 (3)
C17—C18—C19—C20	−0.8 (4)	C13—C12—N5—C10	111.8 (2)
C16—C15—C20—C19	0.7 (3)	C14—C12—N5—C10	−119.6 (2)
O2—C15—C20—C19	176.16 (19)	N4—C11—O2—C15	22.9 (3)
C18—C19—C20—C15	0.1 (4)	N5—C11—O2—C15	−157.54 (18)
C2—C1—N1—N2	−0.1 (2)	C20—C15—O2—C11	62.1 (3)
C10—C1—N1—N2	178.1 (2)	C16—C15—O2—C11	−122.2 (2)
C1—N1—N2—N3	0.3 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13*A*···*Cg*ⁱ	0.96	2.75	3.696 (3)	171

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