organic compounds

3-Phenyl-2-(prop-2-ynyloxy)-1-benzo-furo[3,2-d]pyrimidin-4(3H)-one

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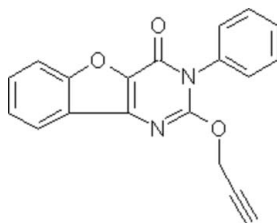Correspondence e-mail: huyangg111@yahoo.com.cn

In the title compound, $C_{19}H_{12}N_2O_3$, the 1-benzofuro[3,2-d]pyrimidinone unit is approximately planar, the maximum deviation from the mean plane being 0.045 (1) Å. The attached phenyl ring makes a dihedral angle of 86.73 (6)° with the fused ring system. The packing of the molecules in the crystal structure is mainly governed by C—H···π hydrogen-bonding interactions.

Related literature

For related preparation and biological activity, see: Bodke & Sangapure (2003). For related literature, see: Ding et al., 2004. For the crystal structures of other fused pyrimidinone derivatives, see: Hu et al. (2005, 2006, 2007).

Experimental

Crystal data

$C_{19}H_{12}N_2O_3$	V = 1542.0 (3) Å³
M_r = 316.31	Z = 4
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
a = 12.6748 (13) Å	μ = 0.09 mm^{-1}
b = 7.1531 (7) Å	T = 292 (2) K
c = 17.5793 (17) Å	0.30 × 0.20 × 0.06 mm
β = 104.645 (2)°	

Data collection

Bruker SMART 4K CCD area-detector diffractometer	9340 measured reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	3496 independent reflections
	2681 reflections with $I > 2\sigma(I)$
T_{min} = 0.972, T_{max} = 0.994	R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046	217 parameters
$wR(F^2)$ = 0.119	H-atom parameters constrained
S = 1.02	$\Delta\rho_{max}$ = 0.16 e Å^{-3}
3496 reflections	$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···$Cg1$[i]	0.93	2.78	3.529 (1)	138
C4—H4···$Cg2$[ii]	0.93	2.81	3.641 (1)	150
C11—H11A···$Cg2$[iii]	0.97	2.76	3.402 (1)	124
C31—H13···$Cg1$[iv]	0.93	2.77	3.521 (1)	139

Symmetry codes: (i) $x + \frac{1}{2}, -y + \frac{3}{2}, z + \frac{1}{2}$; (ii) $-x + \frac{5}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$; (iii) $x, y - 1, z$; (iv) $-x + \frac{3}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$. $Cg1$ is the centroid of the C14–C19 phenyl ring and $Cg2$ is the centroid of the C1–C6 ring.

Data collection: SMART (Bruker, 2001); cell refinement: SAINT-Plus (Bruker, 2001); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: PLATON (Spek, 2003); software used to prepare material for publication: SHELXTL (Sheldrick, 2001).

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supporting information

3-Phenyl-2-(prop-2-ynyloxy)-1-benzofuro[3,2-*d*]pyrimidin-4(3*H*)-one

### Yong-Nian Qu, Long-Rui Pan and Yang-Gen Hu

S1. Comment

Benzofuropyrimidine 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 one such benzofuropyrimidinone derivative. Fig. 1 shows the molecular structure of (I) with the atomic numbering scheme. Bond lengths and angles are unexceptional (Hu *et al.*, 2005, 2006, 2007). The benzofuropyrimidine ring system is almost planar, with a maximum deviation of 0.045 (6) Å for atom C7; the C14—C19 phenyl ring is twisted with respect to it, with a dihedral angle of 86.73 (6)°. In the crystal, intermolecular C—H···π hydrogen bonds (Table 1) stabilize the crystal structure (Fig. 2).

S2. Experimental

To a solution of ethyl 3-((phenylimino)methyleneamino)benzofuran-2-carboxylate (3 mmol) in dichloromethane (5 ml) was added sodium prop-2-yn-1-oxide (3 mmol) in prop-2-yn-1-ol (5 ml). After stirring the reaction mixture for 2 h, the solvent was removed under reduced pressure and the residue was recrystallized from ethanol to give the title compound, in a yield of 89%. Crystals suitable for single-crystal X-ray diffraction were obtained by recrystallization from a mixed solvent of ethanol and dichloromethane (1:1 *v*/*v*) at room temperature.

S3. Refinement

All C-bound H atoms were positioned geometrically, with C—H = 0.93 Å, U_{iso}=1.2U_{eq} (C) for C*sp* and C*sp*^{2}, C—H = 0.97 Å, U_{iso} = 1.2U_{eq} (C) for CH$_2$.
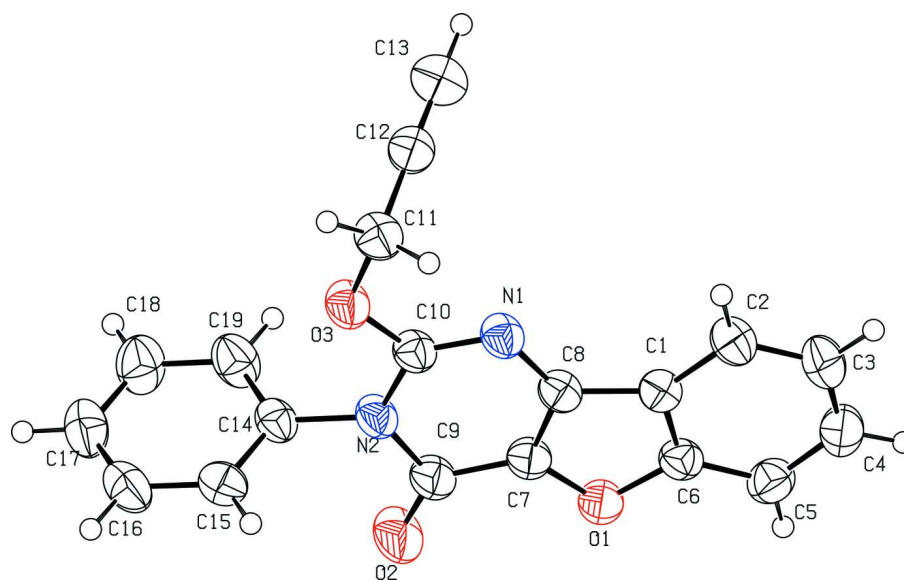
Figure 1

The molecular structure of the title compound, showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.
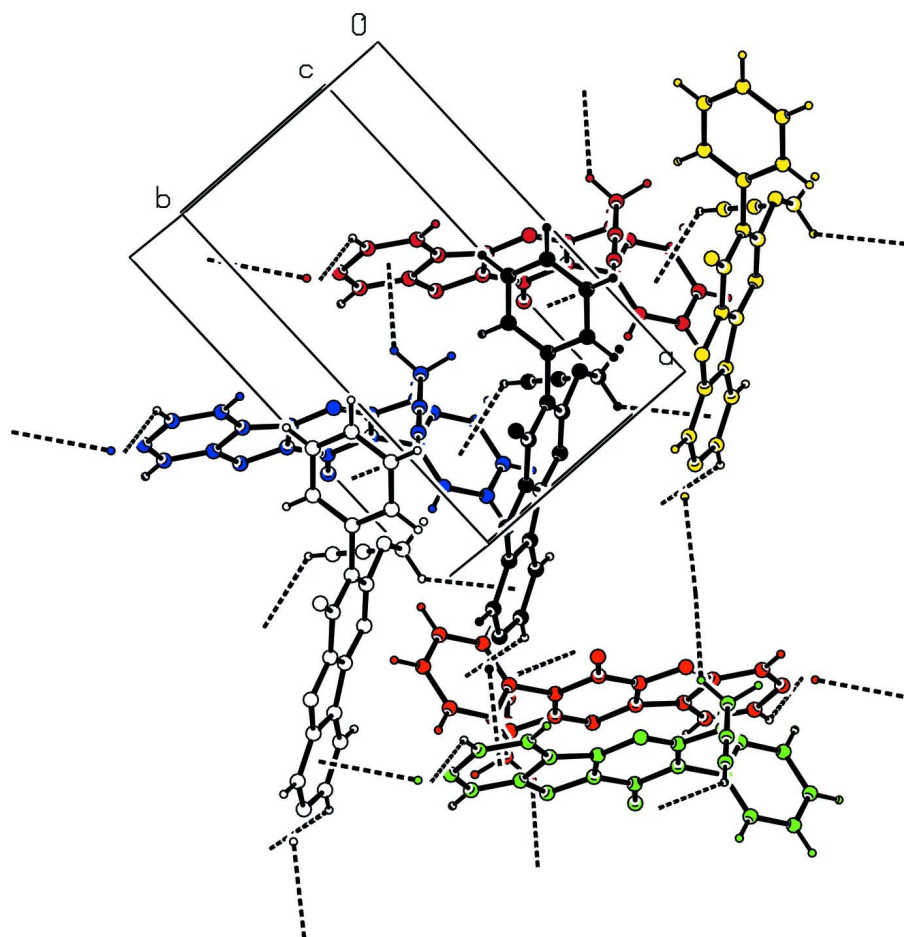
Figure 2

The packing in the crystal structure, showing C—H···π hydrogen bonding interactions as dashed lines.

3-Phenyl-2-(prop-2-ynyloxy)-1-benzofuro[3,2-d]pyrimidin-4(3H)-one

Crystal data

$C_{19}H_{12}N_2O_3$	$F(000) = 656$
$M_r = 316.31$	$D_x = 1.362$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 3101 reflections
$a = 12.6748$ (13) Å	$\theta = 2.4–27.4°$
$b = 7.1531$ (7) Å	$\mu = 0.09$ mm^{-1}
$c = 17.5793$ (17) Å	$T = 292$ K
$\beta = 104.645$ (2)°	Block, colorless
$V = 1542.0$ (3) Å^3	$0.30 \times 0.20 \times 0.06$ mm
$Z = 4$	

Data collection

Bruker SMART 4K CCD area-detector diffractometer	Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
Radiation source: fine-focus sealed tube	$T_{min} = 0.972$, $T_{max} = 0.994$
Graphite monochromator	9340 measured reflections
φ and ω scans	3496 independent reflections
	2681 reflections with $I > 2\sigma(I)$

$R_{int} = 0.041$

$\theta_{max} = 27.5°$, $\theta_{min} = 1.8°$

$h = -8 \rightarrow 16$

$k = -9 \rightarrow 8$

$l = -22 \rightarrow 22$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.046$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.119$	
$S = 1.02$	H-atom parameters constrained
3496 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0641P)^2]$
217 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	$\Delta\rho_{max} = 0.16$ 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.

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	1.05495 (11)	0.81800 (18)	0.22716 (7)	0.0377 (3)
C2	1.11240 (12)	0.85724 (19)	0.30421 (8)	0.0455 (4)
H2	1.1116	0.7745	0.3449	0.055*
C3	1.17039 (12)	1.0220 (2)	0.31838 (9)	0.0510 (4)
H3	1.2099	1.0502	0.3693	0.061*
C4	1.17078 (13)	1.1476 (2)	0.25748 (10)	0.0522 (4)
H4	1.2099	1.2584	0.2691	0.063*
C5	1.11500 (12)	1.1122 (2)	0.18077 (9)	0.0482 (4)
H5	1.1156	1.1953	0.1402	0.058*
C6	1.05806 (11)	0.9455 (2)	0.16777 (7)	0.0403 (3)
C7	0.95602 (11)	0.7144 (2)	0.11079 (7)	0.0409 (3)
C8	0.98690 (11)	0.66798 (18)	0.18824 (7)	0.0380 (3)
C9	0.88390 (12)	0.6046 (2)	0.05294 (8)	0.0454 (4)
C10	0.88737 (11)	0.40745 (19)	0.16784 (7)	0.0397 (3)
C11	0.88258 (13)	0.1884 (2)	0.26800 (8)	0.0467 (4)
H11A	0.9608	0.2064	0.2860	0.056*
H11B	0.8678	0.0561	0.2716	0.056*
C12	0.82912 (12)	0.2919 (2)	0.31909 (8)	0.0456 (4)
C13	0.78913 (15)	0.3726 (2)	0.36209 (10)	0.0625 (5)
H13	0.7572	0.4371	0.3964	0.075*
C14	0.76773 (12)	0.32631 (18)	0.03895 (7)	0.0400 (3)
C15	0.79825 (13)	0.1850 (2)	−0.00388 (8)	0.0468 (4)

H15	0.8715	0.1633	−0.0009	0.056*
C16	0.71813 (15)	0.0755 (2)	−0.05158 (9)	0.0555 (4)
H16	0.7378	−0.0211	−0.0806	0.067*
C17	0.60970 (15)	0.1081 (2)	−0.05642 (9)	0.0583 (4)
H17	0.5563	0.0355	−0.0893	0.070*
C18	0.58085 (13)	0.2486 (3)	−0.01233 (10)	0.0612 (5)
H18	0.5077	0.2693	−0.0146	0.073*
C19	0.65962 (13)	0.3592 (2)	0.03527 (9)	0.0555 (4)
H19	0.6399	0.4551	0.0646	0.067*
N1	0.95387 (9)	0.50832 (16)	0.21918 (6)	0.0416 (3)
N2	0.85008 (9)	0.44489 (16)	0.08854 (6)	0.0413 (3)
O1	0.99762 (8)	0.88383 (13)	0.09524 (5)	0.0461 (3)
O2	0.85057 (11)	0.63467 (16)	−0.01731 (6)	0.0670 (4)
O3	0.84625 (9)	0.24665 (14)	0.18664 (5)	0.0495 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0361 (7)	0.0393 (7)	0.0367 (7)	0.0037 (6)	0.0071 (6)	0.0010 (5)
C2	0.0483 (8)	0.0460 (9)	0.0378 (7)	0.0050 (6)	0.0027 (6)	0.0011 (6)
C3	0.0485 (9)	0.0527 (9)	0.0455 (8)	0.0006 (7)	0.0003 (7)	−0.0085 (7)
C4	0.0470 (9)	0.0486 (9)	0.0597 (9)	−0.0061 (7)	0.0112 (7)	−0.0075 (7)
C5	0.0487 (9)	0.0489 (9)	0.0490 (8)	−0.0044 (7)	0.0161 (7)	0.0043 (7)
C6	0.0378 (7)	0.0472 (8)	0.0356 (7)	0.0017 (6)	0.0087 (6)	−0.0002 (6)
C7	0.0459 (8)	0.0434 (8)	0.0327 (7)	−0.0017 (6)	0.0086 (6)	0.0042 (6)
C8	0.0382 (7)	0.0410 (8)	0.0331 (7)	0.0049 (6)	0.0055 (6)	0.0014 (5)
C9	0.0517 (9)	0.0499 (9)	0.0326 (7)	−0.0026 (7)	0.0070 (6)	0.0031 (6)
C10	0.0450 (8)	0.0407 (7)	0.0319 (7)	0.0003 (6)	0.0070 (6)	0.0028 (6)
C11	0.0588 (9)	0.0415 (8)	0.0377 (7)	0.0021 (7)	0.0082 (7)	0.0091 (6)
C12	0.0475 (9)	0.0474 (9)	0.0390 (8)	−0.0010 (7)	0.0055 (6)	0.0067 (6)
C13	0.0673 (11)	0.0661 (11)	0.0560 (10)	0.0056 (9)	0.0194 (9)	−0.0024 (8)
C14	0.0468 (8)	0.0405 (8)	0.0295 (6)	0.0001 (6)	0.0040 (6)	0.0004 (5)
C15	0.0527 (9)	0.0495 (9)	0.0385 (7)	0.0036 (7)	0.0124 (7)	0.0015 (6)
C16	0.0757 (12)	0.0456 (9)	0.0444 (8)	0.0005 (8)	0.0135 (8)	−0.0092 (7)
C17	0.0628 (11)	0.0528 (10)	0.0509 (9)	−0.0088 (8)	−0.0011 (8)	−0.0049 (7)
C18	0.0433 (9)	0.0667 (11)	0.0666 (11)	0.0016 (8)	0.0009 (8)	−0.0073 (9)
C19	0.0515 (10)	0.0567 (10)	0.0551 (9)	0.0076 (7)	0.0075 (7)	−0.0141 (7)
N1	0.0489 (7)	0.0410 (7)	0.0319 (6)	−0.0009 (5)	0.0048 (5)	0.0028 (5)
N2	0.0475 (7)	0.0443 (7)	0.0290 (5)	−0.0030 (5)	0.0041 (5)	−0.0005 (5)
O1	0.0533 (6)	0.0497 (6)	0.0342 (5)	−0.0078 (5)	0.0087 (4)	0.0047 (4)
O2	0.0928 (9)	0.0695 (8)	0.0301 (5)	−0.0207 (7)	−0.0005 (5)	0.0078 (5)
O3	0.0649 (7)	0.0460 (6)	0.0339 (5)	−0.0101 (5)	0.0058 (5)	0.0040 (4)

Geometric parameters (Å, °)

C1—C6	1.3941 (19)	C10—N2	1.3804 (16)
C1—C2	1.3946 (18)	C11—O3	1.4486 (15)
C1—C8	1.4371 (18)	C11—C12	1.457 (2)

C2—C3	1.378 (2)	C11—H11A	0.9700
C2—H2	0.9300	C11—H11B	0.9700
C3—C4	1.398 (2)	C12—C13	1.164 (2)
C3—H3	0.9300	C13—H13	0.9300
C4—C5	1.379 (2)	C14—C15	1.3731 (19)
C4—H4	0.9300	C14—C19	1.376 (2)
C5—C6	1.383 (2)	C14—N2	1.4522 (17)
C5—H5	0.9300	C15—C16	1.385 (2)
C6—O1	1.3832 (15)	C15—H15	0.9300
C7—C8	1.3593 (18)	C16—C17	1.375 (2)
C7—O1	1.3766 (16)	C16—H16	0.9300
C7—C9	1.4200 (19)	C17—C18	1.374 (2)
C8—N1	1.3749 (16)	C17—H17	0.9300
C9—O2	1.2190 (16)	C18—C19	1.378 (2)
C9—N2	1.4199 (18)	C18—H18	0.9300
C10—N1	1.2888 (17)	C19—H19	0.9300
C10—O3	1.3382 (16)		
C6—C1—C2	119.28 (13)	O3—C11—H11A	109.1
C6—C1—C8	105.01 (11)	C12—C11—H11A	109.1
C2—C1—C8	135.71 (12)	O3—C11—H11B	109.1
C3—C2—C1	118.12 (13)	C12—C11—H11B	109.1
C3—C2—H2	120.9	H11A—C11—H11B	107.9
C1—C2—H2	120.9	C13—C12—C11	177.69 (16)
C2—C3—C4	121.05 (14)	C12—C13—H13	180.0
C2—C3—H3	119.5	C15—C14—C19	121.04 (13)
C4—C3—H3	119.5	C15—C14—N2	119.98 (13)
C5—C4—C3	122.07 (14)	C19—C14—N2	118.98 (12)
C5—C4—H4	119.0	C14—C15—C16	118.90 (15)
C3—C4—H4	119.0	C14—C15—H15	120.6
C4—C5—C6	115.92 (13)	C16—C15—H15	120.6
C4—C5—H5	122.0	C17—C16—C15	120.66 (14)
C6—C5—H5	122.0	C17—C16—H16	119.7
C5—C6—O1	124.85 (12)	C15—C16—H16	119.7
C5—C6—C1	123.55 (12)	C18—C17—C16	119.57 (15)
O1—C6—C1	111.59 (12)	C18—C17—H17	120.2
C8—C7—O1	112.72 (12)	C16—C17—H17	120.2
C8—C7—C9	123.55 (13)	C17—C18—C19	120.47 (16)
O1—C7—C9	123.65 (12)	C17—C18—H18	119.8
C7—C8—N1	124.03 (12)	C19—C18—H18	119.8
C7—C8—C1	106.30 (12)	C14—C19—C18	119.36 (14)
N1—C8—C1	129.65 (12)	C14—C19—H19	120.3
O2—C9—N2	121.50 (13)	C18—C19—H19	120.3
O2—C9—C7	128.57 (14)	C10—N1—C8	113.50 (11)
N2—C9—C7	109.92 (11)	C10—N2—C9	122.46 (11)
N1—C10—O3	122.34 (12)	C10—N2—C14	120.23 (11)
N1—C10—N2	126.51 (13)	C9—N2—C14	117.18 (10)
O3—C10—N2	111.15 (11)	C7—O1—C6	104.37 (10)

O3—C11—C12	112.40 (12)	C10—O3—C11	116.41 (11)
C6—C1—C2—C3	0.0 (2)	C16—C17—C18—C19	1.4 (3)
C8—C1—C2—C3	179.90 (15)	C15—C14—C19—C18	−0.1 (2)
C1—C2—C3—C4	0.7 (2)	N2—C14—C19—C18	179.27 (14)
C2—C3—C4—C5	−0.9 (2)	C17—C18—C19—C14	−0.7 (3)
C3—C4—C5—C6	0.4 (2)	O3—C10—N1—C8	179.94 (12)
C4—C5—C6—O1	−179.66 (13)	N2—C10—N1—C8	0.8 (2)
C4—C5—C6—C1	0.3 (2)	C7—C8—N1—C10	−1.97 (19)
C2—C1—C6—C5	−0.5 (2)	C1—C8—N1—C10	176.24 (13)
C8—C1—C6—C5	179.57 (13)	N1—C10—N2—C9	1.1 (2)
C2—C1—C6—O1	179.48 (12)	O3—C10—N2—C9	−178.16 (12)
C8—C1—C6—O1	−0.48 (14)	N1—C10—N2—C14	−174.64 (13)
O1—C7—C8—N1	178.20 (12)	O3—C10—N2—C14	6.10 (17)
C9—C7—C8—N1	1.4 (2)	O2—C9—N2—C10	179.54 (13)
O1—C7—C8—C1	−0.37 (16)	C7—C9—N2—C10	−1.62 (19)
C9—C7—C8—C1	−177.17 (13)	O2—C9—N2—C14	−4.6 (2)
C6—C1—C8—C7	0.50 (14)	C7—C9—N2—C14	174.25 (12)
C2—C1—C8—C7	−179.45 (15)	C15—C14—N2—C10	−96.71 (16)
C6—C1—C8—N1	−177.95 (13)	C19—C14—N2—C10	83.87 (17)
C2—C1—C8—N1	2.1 (3)	C15—C14—N2—C9	87.32 (15)
C8—C7—C9—O2	179.20 (15)	C19—C14—N2—C9	−92.09 (16)
O1—C7—C9—O2	2.7 (3)	C8—C7—O1—C6	0.08 (15)
C8—C7—C9—N2	0.5 (2)	C9—C7—O1—C6	176.88 (13)
O1—C7—C9—N2	−176.00 (12)	C5—C6—O1—C7	−179.79 (13)
O3—C11—C12—C13	−164 (4)	C1—C6—O1—C7	0.26 (14)
C19—C14—C15—C16	0.3 (2)	N1—C10—O3—C11	−1.5 (2)
N2—C14—C15—C16	−179.10 (12)	N2—C10—O3—C11	177.81 (11)
C14—C15—C16—C17	0.4 (2)	C12—C11—O3—C10	77.20 (16)
C15—C16—C17—C18	−1.2 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···*Cg*1[i]	0.93	2.78	3.529 (1)	138
C4—H4···*Cg*2[ii]	0.93	2.81	3.641 (1)	150
C11—H11*A*···*Cg*2[iii]	0.97	2.76	3.402 (1)	124
C31—H13···*Cg*1[iv]	0.93	2.77	3.521 (1)	139

Symmetry codes: (i) $x+1/2$, $−y+3/2$, $z+1/2$; (ii) $−x+5/2$, $y+1/2$, $−z+1/2$; (iii) x, $y−1$, z; (iv) $−x+3/2$, $y+1/2$, $−z+1/2$.