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2-(2-Hydroxyethylamino)-3-phenyl-1-benzofuro[3,2-*d*]pyrimidin-4(3*H*)-one dichloromethane hemisolvate

Zheng-Hong Zhang,[a,b]* Xiao-Ling Liu[c] and Long-Ju Chen[b]

[a]Department of Neurology, Affiliated Renmin Hospital, Yunyang Medical College, Shiyan 442000, People's Republic of China, [b]Department of Human Anatomy, Yunyang Medical College, Shiyan 442000, People's Republic of China, and [c]Department of Medicinal Chemistry, Yunyang Medical College, Shiyan 442000, People's Republic of China
Correspondence e-mail: zhangzh8875301@yahoo.com.cn

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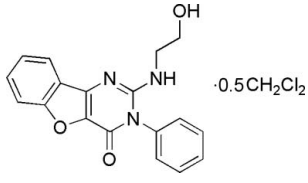
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.005 Å; R factor = 0.066; wR factor = 0.203; data-to-parameter ratio = 13.0.

In the title compound, $C_{18}H_{15}N_3O_3\cdot0.5CH_2Cl_2$, the fused ring benzofuro[2,3-*d*]pyrimidine system is essentially planar [maximum deviation 0.029 (1) Å]. The planes of the pyrimidinone and phenyl rings are nearly perpendicular [dihedral angle = 87.50 (14)°]. The packing of the molecules in the crystal structure is governed mainly by intermolecular O—H···O and N—H···O hydrogen-bonding interactions and intermolecular π–π interactions between benzofuro[3,2-*d*]-pyrimidine units [the interplanar distances are *ca* 3.4 and 3.5 Å, and the distances between adjacent ring centroids are in the range 3.64 (1)–3.76 (1) Å]. The dichloromethane solvent molecule lies on a special position.

Related literature

For the preparation and biological activity of benzofuropyrimidine derivatives, see: Moneam *et al.* (2004); Bodke *et al.* (2003). For π-π stacking interactions, see: Hu *et al.* (2005, 2006, 2007, 2008); Janiak (2000). For the structures of other fused pyrimidinone derivatives, see: Hu *et al.* (2005, 2006, 2007, 2008).



Experimental

Crystal data

$C_{18}H_{15}N_3O_3\cdot0.5CH_2Cl_2$
M_r = 363.80
Monoclinic, $C2/c$
a = 26.928 (2) Å
b = 7.8931 (7) Å
c = 17.3134 (15) Å
β = 110.638 (2)°
V = 3443.7 (5) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.25 mm^{-1}
T = 292 K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.941, T_{max} = 0.960
6773 measured reflections
3008 independent reflections
2321 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.203
S = 1.04
3008 reflections
232 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.74 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3B···O3^{i}	0.86	2.23	2.903 (3)	136
O3—H3A···O2^{ii}	0.82	1.94	2.744 (3)	167

Symmetry codes: (i) $-x+\frac{1}{2}, -y+\frac{3}{2}, -z$; (ii) $x, -y+2, z-\frac{1}{2}$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; 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: AT2780).

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supporting information

Acta Cryst. (2009). E**65**, o1330 [doi:10.1107/S1600536809017814]

2-(2-Hydroxyethylamino)-3-phenyl-1-benzofuro[3,2-*d*]pyrimidin-4(3*H*)-one dichloromethane hemisolvate

Zheng-Hong Zhang, Xiao-Ling Liu and Long-Ju Chen

S1. Comment

Derivatives of benzofuropyrimidines are of great importance because of their remarkable biological properties, such as the interesting analgesic, antihypertensive, antipyretic, antiviral, and anti-inflammatory activities (Moneam *et al.*, 2004 and Bodke *et al.*, 2003). Some X-ray crystal structures of benzofuro[3,2-*d*]pyrimidinone derivatives have been reported (Hu *et al.*, 2005, 2006, 2007, 2008). The heterocyclic title compound (I) may be used as a new precursor for obtaining bioactive molecules and its structure is presented here (Fig.1).

In the molecule of (I), all ring atoms of benzofuro[2,3-*d*]pyrimidine system are essentially coplanar, with maximum deviations -0.029 (1)Å and 0.027 (2) Å for C7 and N2, respectively. The pyrimidinone ring and the phenyl (C14—C19) ring are nearly perpendicular [dihedral angle = 87.50 (14)]. Intermolecular O—H···O and N—H···O hydrogen-bonding interactions (Table 1) link the molecules, helping to stabilize the crystal structure. Further stability the crystal structure is provided by offset π-π stacking interactions (Janiak, 2000) involving the fused benzofuro[2,3-*d*]pyrimidin system moeties. The interplanar distance are *ca* 3.5 Å, with distances between adjacent ring centroids of 3.6 (1)–3.8 (1)Å [symmetry code relating the adjacent rings: -*x*, 2 - *y*, -*z*].

S2. Experimental

For background references, see: Hu *et al.* (2008).

S3. Refinement

All H atoms were located in difference maps and treated as riding atoms with C—H = 0.93 Å, U_{iso}=1.2U_{eq} (C) for Csp^2, C—H = 0.97 Å, U_{iso} = 1.2U_{eq} (C) for CH_2, O—H = 0.82 Å, U_{iso} = 1.2U_{eq} (C) for OH, N—H = 0.86 Å, U_{iso} = 1.2U_{eq} (N) for NH.

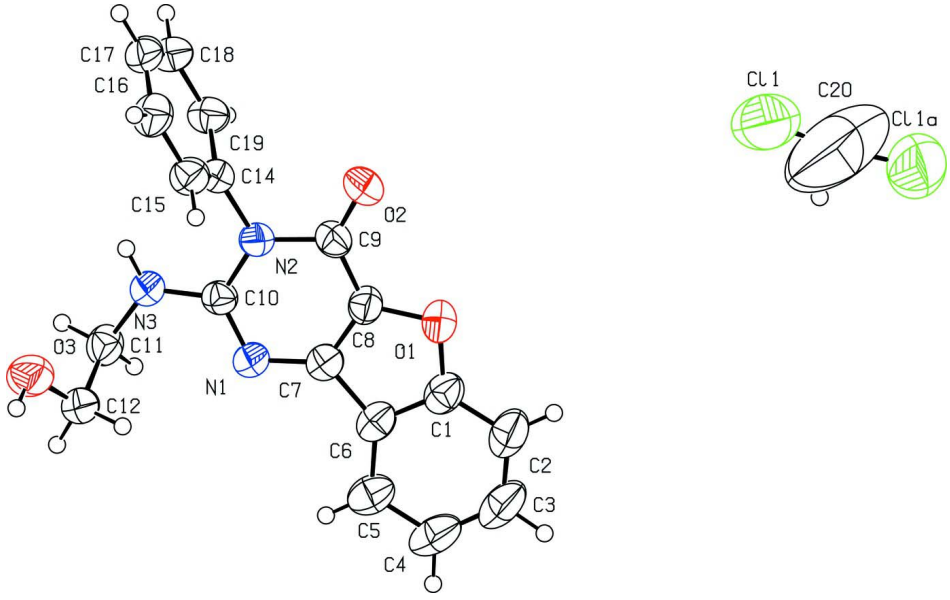

Figure 1

View of the molecular structure of the title compound, showing the atom labelling scheme and with displacement ellipsoids drawn at 50% probability level. [Symmetry code: (a) -x, y, -z +3/2].

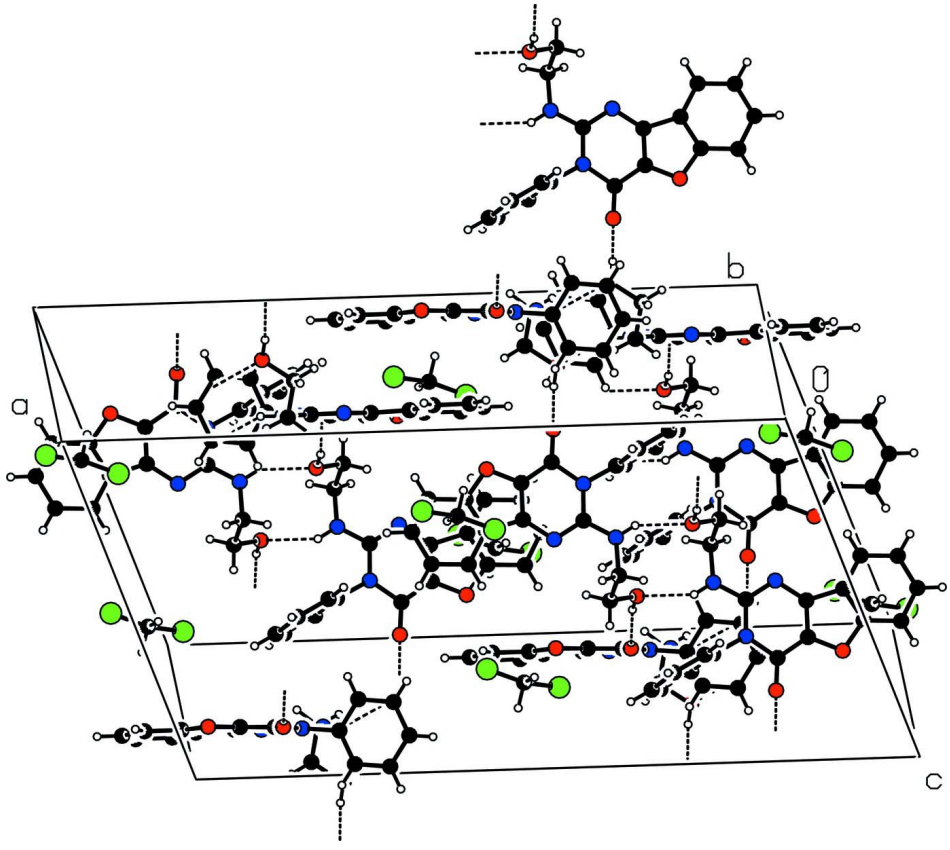

Figure 2

A partial view of the crystal packing of the title compound, showing the hydrogen-bonded stacking interactions (dashed lines).

2-(2-Hydroxyethylamino)-3-phenyl-1-benzofuro[3,2-*d*]pyrimidin- 4(3*H*)-one dichloromethane hemisolvate

Crystal data

$C_{18}H_{15}N_3O_3 \cdot 0.5CH_2Cl_2$
$M_r = 363.80$
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
$a = 26.928$ (2) Å
$b = 7.8931$ (7) Å
$c = 17.3134$ (15) Å
$\beta = 110.638$ (2)°
$V = 3443.7$ (5) Å^3
$Z = 8$
$F(000) = 1512$
$D_x = 1.403$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2289 reflections
$\theta = 2.5$–25.0°
$\mu = 0.25$ mm^{-1}
$T = 292$ K
Needle, colourless
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{min} = 0.941$, $T_{max} = 0.960$
6773 measured reflections
3008 independent reflections
2321 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.5°$
$h = -24 \rightarrow 32$
$k = -9 \rightarrow 9$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.066$
$wR(F^2) = 0.203$
$S = 1.04$
3008 reflections
232 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
$w = 1/[\sigma^2(F_o^2) + (0.1003P)^2 + 4.9568P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.74$ e Å^{-3}
$\Delta\rho_{min} = -0.46$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0023 (4)

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}	Occ. (<1)
C1	0.00474 (12)	0.9366 (4)	0.1209 (2)	0.0562 (8)	
C2	−0.04614 (14)	0.9437 (5)	0.1234 (2)	0.0724 (10)	
H2	−0.0549	1.0163	0.1589	0.087*	

C3	−0.08262 (14)	0.8376 (6)	0.0704 (3)	0.0828 (13)	
H3	−0.1172	0.8374	0.0703	0.099*	
C4	−0.06967 (14)	0.7306 (6)	0.0171 (3)	0.0772 (11)	
H4	−0.0958	0.6618	−0.0185	0.093*	
C5	−0.01884 (12)	0.7234 (4)	0.0155 (2)	0.0626 (9)	
H5	−0.0103	0.6509	−0.0203	0.075*	
C6	0.01922 (11)	0.8287 (4)	0.06958 (18)	0.0502 (7)	
C7	0.07480 (11)	0.8619 (4)	0.08694 (17)	0.0456 (7)	
C8	0.08819 (11)	0.9878 (4)	0.14460 (18)	0.0494 (7)	
C9	0.13833 (11)	1.0657 (4)	0.17189 (17)	0.0488 (7)	
C10	0.15717 (11)	0.8521 (3)	0.08219 (16)	0.0423 (7)	
C11	0.18301 (12)	0.6367 (4)	0.0038 (2)	0.0534 (8)	
H11A	0.1605	0.5601	0.0205	0.064*	
H11B	0.2159	0.5778	0.0106	0.064*	
C12	0.15587 (12)	0.6799 (5)	−0.0862 (2)	0.0617 (9)	
H12A	0.1455	0.5770	−0.1185	0.074*	
H12B	0.1242	0.7464	−0.0936	0.074*	
C14	0.22429 (10)	1.0652 (4)	0.15552 (16)	0.0443 (7)	
C15	0.23170 (12)	1.1918 (4)	0.10617 (18)	0.0525 (8)	
H15	0.2036	1.2268	0.0597	0.063*	
C16	0.28099 (13)	1.2672 (4)	0.1257 (2)	0.0591 (8)	
H16	0.2862	1.3529	0.0925	0.071*	
C17	0.32232 (12)	1.2151 (4)	0.1946 (2)	0.0577 (8)	
H17	0.3555	1.2653	0.2078	0.069*	
C18	0.31458 (12)	1.0894 (4)	0.2437 (2)	0.0603 (9)	
H18	0.3426	1.0553	0.2903	0.072*	
C19	0.26543 (12)	1.0123 (4)	0.22476 (19)	0.0533 (8)	
H19	0.2603	0.9267	0.2581	0.064*	
Cl1	0.04437 (10)	0.5409 (4)	0.71999 (15)	0.1632 (11)	
N1	0.10909 (9)	0.7873 (3)	0.05548 (14)	0.0463 (6)	
N2	0.17227 (9)	0.9896 (3)	0.13565 (14)	0.0439 (6)	
N3	0.19460 (9)	0.7832 (3)	0.05727 (14)	0.0495 (6)	
H3B	0.2259	0.8269	0.0733	0.059*	
O1	0.04639 (8)	1.0374 (3)	0.16786 (13)	0.0602 (6)	
O2	0.15384 (9)	1.1865 (3)	0.21917 (14)	0.0665 (7)	
O3	0.19168 (9)	0.7736 (4)	−0.11261 (14)	0.0768 (8)	
H3A	0.1774	0.7980	−0.1615	0.115*	
C20	0.0000	0.509 (3)	0.7500	0.394 (18)	
H20A	0.0194	0.4328	0.7943	0.473*	0.5
H20B	−0.0194	0.4329	0.7057	0.473*	0.5

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0478 (17)	0.068 (2)	0.0549 (18)	0.0005 (15)	0.0201 (14)	0.0145 (16)
C2	0.053 (2)	0.099 (3)	0.073 (2)	0.011 (2)	0.0313 (18)	0.018 (2)
C3	0.0431 (19)	0.120 (3)	0.087 (3)	−0.001 (2)	0.0251 (19)	0.029 (3)
C4	0.0456 (19)	0.093 (3)	0.084 (3)	−0.0150 (18)	0.0124 (18)	0.017 (2)

C5	0.0516 (18)	0.061 (2)	0.070 (2)	−0.0065 (15)	0.0149 (16)	0.0112 (17)
C6	0.0435 (16)	0.0517 (17)	0.0555 (17)	0.0010 (13)	0.0178 (13)	0.0140 (14)
C7	0.0438 (15)	0.0473 (16)	0.0449 (15)	−0.0002 (12)	0.0148 (12)	0.0062 (13)
C8	0.0437 (16)	0.0604 (18)	0.0476 (16)	0.0026 (13)	0.0203 (13)	0.0019 (14)
C9	0.0524 (17)	0.0546 (18)	0.0395 (15)	0.0007 (14)	0.0164 (13)	−0.0018 (14)
C10	0.0435 (15)	0.0447 (15)	0.0380 (14)	−0.0031 (12)	0.0134 (11)	0.0018 (12)
C11	0.0513 (17)	0.0456 (16)	0.068 (2)	−0.0010 (13)	0.0265 (15)	−0.0059 (15)
C12	0.0446 (17)	0.073 (2)	0.065 (2)	−0.0032 (15)	0.0161 (15)	−0.0223 (17)
C14	0.0429 (15)	0.0483 (16)	0.0417 (15)	−0.0034 (12)	0.0149 (12)	−0.0063 (13)
C15	0.0495 (17)	0.0603 (19)	0.0460 (16)	−0.0003 (14)	0.0149 (13)	0.0063 (14)
C16	0.0593 (19)	0.0572 (19)	0.067 (2)	−0.0058 (15)	0.0294 (16)	0.0038 (16)
C17	0.0450 (17)	0.0612 (19)	0.069 (2)	−0.0117 (14)	0.0225 (15)	−0.0185 (17)
C18	0.0444 (17)	0.073 (2)	0.0546 (18)	−0.0015 (15)	0.0068 (14)	−0.0076 (17)
C19	0.0525 (18)	0.0566 (18)	0.0469 (17)	−0.0055 (14)	0.0126 (14)	0.0013 (14)
Cl1	0.1220 (17)	0.241 (3)	0.1193 (16)	−0.0455 (18)	0.0331 (14)	−0.0050 (18)
N1	0.0406 (13)	0.0489 (14)	0.0493 (13)	−0.0041 (10)	0.0158 (10)	−0.0024 (11)
N2	0.0413 (13)	0.0491 (14)	0.0412 (12)	−0.0043 (10)	0.0142 (10)	−0.0030 (11)
N3	0.0408 (13)	0.0573 (15)	0.0520 (14)	−0.0054 (11)	0.0182 (11)	−0.0109 (12)
O1	0.0528 (13)	0.0745 (15)	0.0603 (13)	0.0037 (11)	0.0286 (11)	−0.0056 (11)
O2	0.0653 (14)	0.0744 (16)	0.0605 (13)	−0.0098 (12)	0.0229 (11)	−0.0266 (12)
O3	0.0628 (15)	0.110 (2)	0.0520 (13)	−0.0030 (14)	0.0131 (11)	0.0062 (13)
C20	0.137 (13)	0.56 (5)	0.44 (4)	0.000	0.038 (18)	0.000

Geometric parameters (Å, º)

C1—O1	1.381 (4)	C11—H11A	0.9700
C1—C6	1.383 (5)	C11—H11B	0.9700
C1—C2	1.387 (5)	C12—O3	1.413 (4)
C2—C3	1.369 (6)	C12—H12A	0.9700
C2—H2	0.9300	C12—H12B	0.9700
C3—C4	1.383 (6)	C14—C15	1.375 (4)
C3—H3	0.9300	C14—C19	1.379 (4)
C4—C5	1.380 (5)	C14—N2	1.448 (3)
C4—H4	0.9300	C15—C16	1.383 (4)
C5—C6	1.393 (4)	C15—H15	0.9300
C5—H5	0.9300	C16—C17	1.376 (5)
C6—C7	1.443 (4)	C16—H16	0.9300
C7—N1	1.360 (3)	C17—C18	1.370 (5)
C7—C8	1.364 (4)	C17—H17	0.9300
C8—O1	1.379 (3)	C18—C19	1.387 (4)
C8—C9	1.405 (4)	C18—H18	0.9300
C9—O2	1.230 (4)	C19—H19	0.9300
C9—N2	1.412 (4)	Cl1—C20	1.483 (5)
C10—N1	1.315 (3)	N3—H3B	0.8600
C10—N3	1.343 (3)	O3—H3A	0.8200
C10—N2	1.391 (3)	C20—H20A	0.9700
C11—N3	1.445 (4)	C20—H20B	0.9700
C11—C12	1.508 (5)		

O1—C1—C6	112.2 (3)	C11—C12—H12A	110.0
O1—C1—C2	124.3 (3)	O3—C12—H12B	110.0
C6—C1—C2	123.4 (3)	C11—C12—H12B	110.0
C3—C2—C1	116.0 (4)	H12A—C12—H12B	108.4
C3—C2—H2	122.0	C15—C14—C19	120.8 (3)
C1—C2—H2	122.0	C15—C14—N2	119.5 (2)
C2—C3—C4	122.1 (3)	C19—C14—N2	119.7 (3)
C2—C3—H3	119.0	C14—C15—C16	119.8 (3)
C4—C3—H3	119.0	C14—C15—H15	120.1
C5—C4—C3	121.6 (4)	C16—C15—H15	120.1
C5—C4—H4	119.2	C17—C16—C15	119.8 (3)
C3—C4—H4	119.2	C17—C16—H16	120.1
C4—C5—C6	117.5 (4)	C15—C16—H16	120.1
C4—C5—H5	121.2	C18—C17—C16	120.1 (3)
C6—C5—H5	121.2	C18—C17—H17	120.0
C1—C6—C5	119.5 (3)	C16—C17—H17	120.0
C1—C6—C7	105.1 (3)	C17—C18—C19	120.8 (3)
C5—C6—C7	135.4 (3)	C17—C18—H18	119.6
N1—C7—C8	124.5 (3)	C19—C18—H18	119.6
N1—C7—C6	129.7 (3)	C14—C19—C18	118.7 (3)
C8—C7—C6	105.8 (3)	C14—C19—H19	120.7
C7—C8—O1	112.8 (3)	C18—C19—H19	120.7
C7—C8—C9	122.7 (3)	C10—N1—C7	114.5 (2)
O1—C8—C9	124.3 (3)	C10—N2—C9	123.0 (2)
O2—C9—C8	128.6 (3)	C10—N2—C14	120.7 (2)
O2—C9—N2	120.3 (3)	C9—N2—C14	116.3 (2)
C8—C9—N2	111.1 (3)	C10—N3—C11	120.8 (2)
N1—C10—N3	119.1 (3)	C10—N3—H3B	119.6
N1—C10—N2	123.9 (2)	C11—N3—H3B	119.6
N3—C10—N2	116.9 (2)	C8—O1—C1	104.0 (2)
N3—C11—C12	113.4 (3)	C12—O3—H3A	109.5
N3—C11—H11A	108.9	Cl1—C20—Cl1^{i}	161 (2)
C12—C11—H11A	108.9	Cl1—C20—H20A	96.0
N3—C11—H11B	108.9	Cl1^{i}—C20—H20A	96.0
C12—C11—H11B	108.9	Cl1—C20—H20B	96.0
H11A—C11—H11B	107.7	Cl1^{i}—C20—H20B	96.0
O3—C12—C11	108.4 (2)	H20A—C20—H20B	103.4
O3—C12—H12A	110.0		

O1—C1—C2—C3	178.0 (3)	C16—C17—C18—C19	0.4 (5)
C6—C1—C2—C3	−0.8 (5)	C15—C14—C19—C18	−0.1 (5)
C1—C2—C3—C4	−0.5 (6)	N2—C14—C19—C18	−178.4 (3)
C2—C3—C4—C5	1.0 (6)	C17—C18—C19—C14	−0.2 (5)
C3—C4—C5—C6	−0.2 (5)	N3—C10—N1—C7	177.5 (2)
O1—C1—C6—C5	−177.3 (3)	N2—C10—N1—C7	−2.4 (4)
C2—C1—C6—C5	1.6 (5)	C8—C7—N1—C10	−3.2 (4)
O1—C1—C6—C7	1.3 (3)	C6—C7—N1—C10	177.5 (3)

C2—C1—C6—C7	−179.8 (3)	N1—C10—N2—C9	5.1 (4)
C4—C5—C6—C1	−1.0 (5)	N3—C10—N2—C9	−174.8 (2)
C4—C5—C6—C7	−179.1 (3)	N1—C10—N2—C14	−173.4 (3)
C1—C6—C7—N1	177.8 (3)	N3—C10—N2—C14	6.7 (4)
C5—C6—C7—N1	−3.9 (6)	O2—C9—N2—C10	179.6 (3)
C1—C6—C7—C8	−1.6 (3)	C8—C9—N2—C10	−1.9 (4)
C5—C6—C7—C8	176.7 (3)	O2—C9—N2—C14	−1.9 (4)
N1—C7—C8—O1	−178.1 (2)	C8—C9—N2—C14	176.7 (2)
C6—C7—C8—O1	1.4 (3)	C15—C14—N2—C10	88.1 (3)
N1—C7—C8—C9	6.4 (5)	C19—C14—N2—C10	−93.5 (3)
C6—C7—C8—C9	−174.1 (3)	C15—C14—N2—C9	−90.5 (3)
C7—C8—C9—O2	175.0 (3)	C19—C14—N2—C9	87.9 (3)
O1—C8—C9—O2	0.0 (5)	N1—C10—N3—C11	−1.8 (4)
C7—C8—C9—N2	−3.5 (4)	N2—C10—N3—C11	178.1 (2)
O1—C8—C9—N2	−178.4 (3)	C12—C11—N3—C10	82.1 (3)
N3—C11—C12—O3	66.0 (3)	C7—C8—O1—C1	−0.6 (3)
C19—C14—C15—C16	0.2 (5)	C9—C8—O1—C1	174.8 (3)
N2—C14—C15—C16	178.6 (3)	C6—C1—O1—C8	−0.5 (3)
C14—C15—C16—C17	−0.1 (5)	C2—C1—O1—C8	−179.4 (3)
C15—C16—C17—C18	−0.2 (5)		

Symmetry code: (i) $-x$, y, $-z+3/2$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*B*···O3^{ii}	0.86	2.23	2.903 (3)	136
O3—H3*A*···O2^{iii}	0.82	1.94	2.744 (3)	167

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