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

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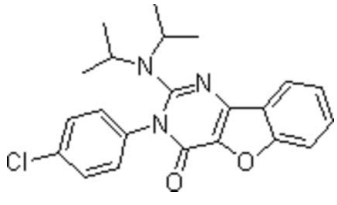
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.005 Å; R factor = 0.049; wR factor = 0.139; data-to-parameter ratio = 15.2.

In the molecule of the title compound, $C_{22}H_{22}ClN_3O_2$, the three fused rings of the benzofuro[3,2-*d*]pyrimidine system are almost coplanar. This ring system is oriented with respect to the substituted benzene ring at a dihedral angle of 79.05 (3)°. Intramolecular C—H···N hydrogen bonding results in the formation of a six-membered ring. In the crystal structure, π–π stacking interactions involving the furan, pyrimidinone and benzene rings are present [centroid-to-centroid distances in the range 3.258 (1)–3.870 (1) Å].

Related literature

For general background, see: Bodke & Sangapure (2003); Ding *et al.* (2004); Janiak (2000). For a related structure, see: Liu *et al.* (2006). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{22}H_{22}ClN_3O_2$
M_r = 395.88
Monoclinic, *Cc*
a = 11.3713 (7) Å
b = 23.2686 (10) Å
c = 7.8405 (5) Å
β = 105.994 (1)°
V = 1994.2 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 295 (2) K
0.20 × 0.10 × 0.10 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.958, T_{max} = 0.979
6825 measured reflections
3919 independent reflections
3221 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.139
S = 1.14
3919 reflections
257 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}
Absolute structure: Flack (1983), with 1735 Friedel pairs
Flack parameter: −0.01 (9)

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

D—H···A	D—H	H···A	D···A	D—H···A
C15—H15A···N2	0.96	2.44	2.946 (5)	113

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* (Bruker, 2001).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2383).

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supporting information

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

Quan-Bin Liao, Gui-Hua Li, Zheng-Rong Zhu and Ming-Guo Liu

S1. Comment

The derivatives of benzofuropyrimidines are of great importance because of their remarkable biological properties (Bodke & Sangapure, 2003). In recent years, we have been engaged in the preparation of derivatives of heterocycles using an aza-Wittig reaction (Ding *et al.*, 2004). The heterocyclic title compound, (I), may be used as a new precursor for obtaining bioactive molecules, and we report herein its crystal structure.

In the molecule of the title compound, (I), (Fig. 1) the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). They are also in agreement with the corresponding values in a reported similar compound (Liu *et al.*, 2006). The three fused rings, A (N1/N2/C7–C10), B (O2/C8/C9/C17/C22) and C (C17–C22), of the benzofuro[3,2-*d*]pyrimidine system are almost co-planar, with a maximum deviation of 0.029 (3) Å (for C17). The co-planar ring system is oriented with respect to the substituted benzene ring D (C1–C6) at a dihedral angle of 79.05 (3)°. The intramolecular C—H···O hydrogen bond (Table 1) results in the formation of a six-membered ring.

Intermolecular π–π stacking interactions (Janiak, 2000) involving the furan, pyrimidinone and benzene rings seem to be effective in stabilizing the crystal structure (Fig. 2). The furan:furan and furan:pyrimidinone interplanar distances are 3.728 (1) Å and 3.510 (1) Å, while the distances between the adjacent ring centroids are 3.870 (1) Å and 3.744 (1) Å [symmetry code: x, 1 - y, -1/2 + z], respectively. A further interaction occurs between the two adjacent furan and benzene rings [symmetry code: x, 1 - y, 1/2 + z] with an interplanar distance of 3.258 (1) Å and a centroid-to-centroid distance of 3.870 (1) Å.

S2. Experimental

For the preparation of the title compound, diisopropylamine (3 mmol) was added to a solution of ethyl 3-((4-chlorophenylimino)methyleneamino)-benzofuran-2-carboxylate (3 mmol) in dichloromethane (5 ml). After stirring the reaction mixture for 1 h, the solvent was removed and anhydrous ethanol (10 ml) with several drops of EtONa in EtOH was added. The mixture was stirred for 2 h at room temperature. The solution was concentrated under reduced pressure and the residue was recrystallized from ethanol to give the title compound (yield; 82%). Single crystals suitable for X-ray analysis were obtained by recrystallization from a mixed solvent of ethanol and dichloromethane (1:1 *v*/*v*) at room temperature.

S3. Refinement

H atoms were positioned geometrically, with C—H = 0.93, 0.98 and 0.96 Å, for aromatic, methine and methyl H atoms and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C), where x = 1.6 for methyl H, and x = 1.5 for all other H atoms.

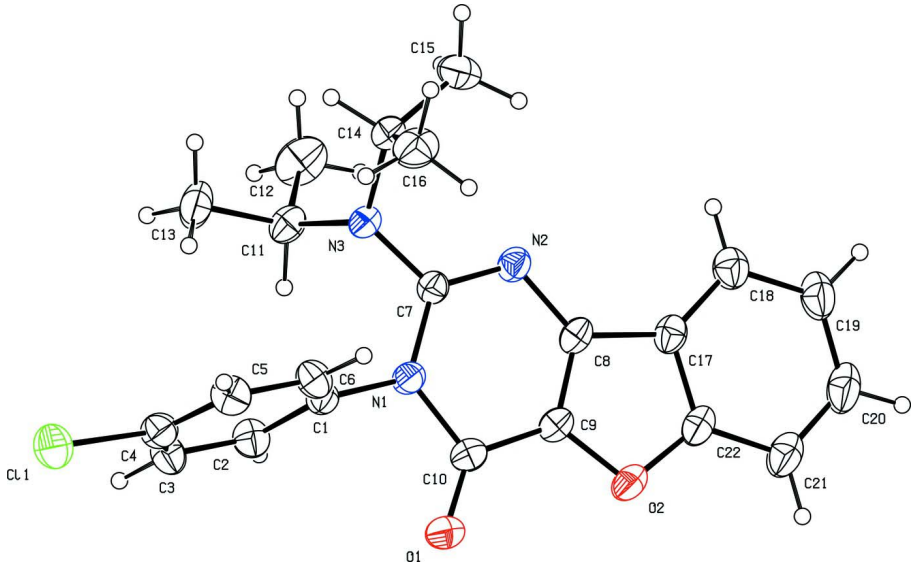

Figure 1

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level

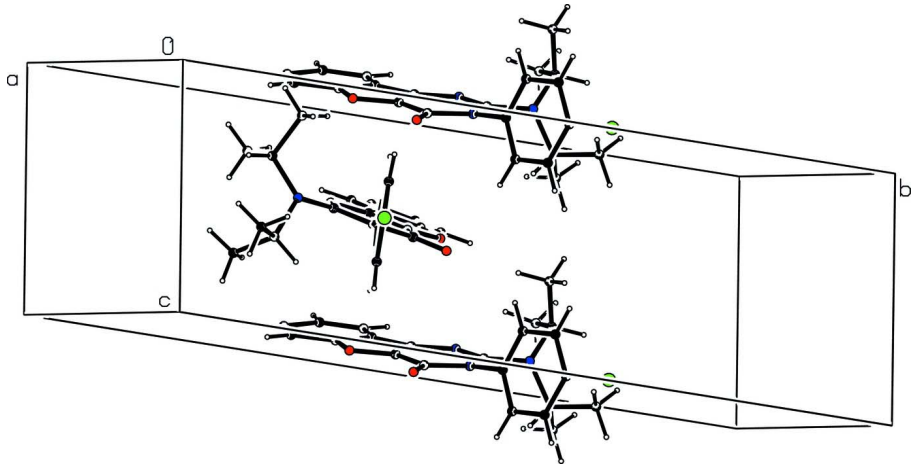

Figure 2

A packing diagram of (I).

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

Crystal data

$C_{22}H_{22}ClN_3O_2$
$M_r = 395.88$
Monoclinic, *Cc*
Hall symbol: C -2yc
$a = 11.3713\ (7)$ Å
$b = 23.2686\ (10)$ Å
$c = 7.8405\ (5)$ Å
$\beta = 105.994\ (1)°$
$V = 1994.2\ (2)$ Å^3
$Z = 4$

$F(000) = 832$
$D_x = 1.319$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3139 reflections
$\theta = 2.7–26.0°$
$\mu = 0.21$ mm^{-1}
$T = 295$ K
Block, blue
0.20 × 0.10 × 0.10 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} = 0.958, T_{max} = 0.979
6825 measured reflections
3919 independent reflections
3221 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 27.0°, θ_{min} = 1.8°
h = −14→14
k = −26→29
l = −9→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.139
S = 1.14
3919 reflections
257 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.059P)^2 + 1.0112P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}
Absolute structure: Flack (1983), with 1735 Friedel pairs
Absolute structure parameter: −0.01 (9)

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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
Cl1	0.25733 (9)	0.34136 (4)	0.47013 (15)	0.0711 (3)
O1	0.6847 (2)	0.52195 (10)	0.5144 (4)	0.0575 (6)
O2	0.9123 (2)	0.56254 (9)	0.4447 (3)	0.0529 (6)
N1	0.7409 (2)	0.43085 (11)	0.4491 (4)	0.0413 (6)
N2	0.9243 (2)	0.41095 (11)	0.3704 (3)	0.0431 (6)
N3	0.7909 (2)	0.33618 (10)	0.3863 (3)	0.0409 (6)
C1	0.6217 (3)	0.41096 (13)	0.4567 (4)	0.0400 (7)
C2	0.5982 (3)	0.40193 (15)	0.6176 (4)	0.0505 (8)
H2	0.6582	0.4099	0.7224	0.061*
C3	0.4858 (3)	0.38108 (16)	0.6236 (5)	0.0541 (8)
H3	0.4694	0.3744	0.7317	0.065*
C4	0.3987 (3)	0.37038 (14)	0.4665 (5)	0.0498 (8)
C5	0.4187 (3)	0.38198 (15)	0.3056 (5)	0.0524 (8)
H5	0.3571	0.3759	0.2011	0.063*
C6	0.5316 (3)	0.40281 (15)	0.3004 (5)	0.0487 (8)

H6	0.5465	0.4112	0.1923	0.058*
C7	0.8236 (3)	0.39358 (12)	0.4014 (4)	0.0383 (6)
C8	0.9451 (3)	0.46920 (13)	0.3863 (4)	0.0435 (7)
C9	0.8700 (3)	0.50707 (13)	0.4357 (4)	0.0436 (7)
C10	0.7588 (3)	0.49109 (13)	0.4729 (4)	0.0440 (7)
C11	0.7984 (3)	0.30526 (14)	0.5543 (4)	0.0488 (8)
H11	0.7911	0.3343	0.6414	0.059*
C12	0.9206 (4)	0.2748 (2)	0.6309 (7)	0.0820 (14)
H12A	0.9271	0.2429	0.5563	0.123*
H12B	0.9252	0.2611	0.7480	0.123*
H12C	0.9864	0.3012	0.6365	0.123*
C13	0.6927 (4)	0.26389 (17)	0.5353 (6)	0.0696 (11)
H13A	0.6169	0.2838	0.4871	0.104*
H13B	0.6944	0.2485	0.6496	0.104*
H13C	0.6997	0.2331	0.4572	0.104*
C14	0.8065 (3)	0.30269 (14)	0.2347 (4)	0.0490 (8)
H14	0.7785	0.2637	0.2498	0.059*
C15	0.9372 (4)	0.2964 (2)	0.2164 (7)	0.0784 (13)
H15A	0.9655	0.3330	0.1872	0.118*
H15B	0.9372	0.2693	0.1242	0.118*
H15C	0.9905	0.2830	0.3266	0.118*
C16	0.7213 (5)	0.32524 (17)	0.0659 (5)	0.0676 (11)
H16A	0.6384	0.3222	0.0721	0.101*
H16B	0.7309	0.3031	−0.0328	0.101*
H16C	0.7401	0.3648	0.0504	0.101*
C17	1.0477 (3)	0.50223 (14)	0.3637 (4)	0.0451 (7)
C18	1.1556 (3)	0.49026 (17)	0.3222 (5)	0.0557 (9)
H18	1.1752	0.4529	0.2984	0.067*
C19	1.2333 (4)	0.53513 (19)	0.3170 (6)	0.0678 (11)
H19	1.3052	0.5281	0.2859	0.081*
C20	1.2061 (4)	0.59093 (19)	0.3576 (6)	0.0714 (12)
H20	1.2615	0.6202	0.3564	0.086*
C21	1.0995 (4)	0.60384 (17)	0.3995 (5)	0.0634 (10)
H21	1.0807	0.6412	0.4252	0.076*
C22	1.0216 (3)	0.55846 (14)	0.4014 (4)	0.0494 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0476 (4)	0.0739 (6)	0.0964 (7)	−0.0115 (5)	0.0277 (5)	−0.0074 (6)
O1	0.0599 (15)	0.0418 (13)	0.0756 (17)	0.0038 (11)	0.0269 (13)	−0.0060 (12)
O2	0.0596 (14)	0.0342 (11)	0.0651 (15)	−0.0081 (10)	0.0176 (12)	−0.0037 (10)
N1	0.0410 (14)	0.0345 (12)	0.0480 (14)	−0.0007 (11)	0.0119 (11)	−0.0010 (11)
N2	0.0395 (13)	0.0377 (13)	0.0508 (16)	−0.0042 (11)	0.0102 (12)	−0.0008 (11)
N3	0.0441 (13)	0.0328 (12)	0.0461 (14)	−0.0028 (11)	0.0131 (11)	−0.0016 (11)
C1	0.0376 (15)	0.0366 (15)	0.0456 (17)	−0.0016 (13)	0.0109 (13)	−0.0016 (12)
C2	0.0508 (19)	0.0566 (19)	0.0427 (18)	−0.0042 (15)	0.0105 (15)	−0.0022 (15)
C3	0.053 (2)	0.065 (2)	0.0477 (18)	−0.0045 (17)	0.0206 (16)	−0.0007 (16)

C4	0.0385 (16)	0.0467 (18)	0.064 (2)	0.0016 (14)	0.0128 (15)	−0.0021 (16)
C5	0.0418 (17)	0.062 (2)	0.0478 (19)	−0.0003 (16)	0.0028 (14)	−0.0029 (16)
C6	0.0452 (17)	0.059 (2)	0.0419 (17)	0.0010 (15)	0.0120 (14)	0.0016 (14)
C7	0.0386 (15)	0.0362 (14)	0.0397 (15)	−0.0001 (12)	0.0099 (12)	0.0020 (12)
C8	0.0438 (16)	0.0359 (15)	0.0469 (17)	−0.0072 (13)	0.0058 (14)	0.0006 (13)
C9	0.0461 (16)	0.0356 (15)	0.0463 (17)	−0.0039 (13)	0.0078 (14)	−0.0018 (13)
C10	0.0466 (15)	0.0378 (15)	0.0456 (17)	0.0034 (15)	0.0091 (13)	0.0001 (14)
C11	0.0548 (18)	0.0403 (17)	0.0467 (17)	−0.0010 (14)	0.0063 (15)	0.0053 (13)
C12	0.079 (3)	0.071 (3)	0.080 (3)	0.011 (2)	−0.005 (2)	0.013 (2)
C13	0.083 (3)	0.055 (2)	0.075 (3)	−0.021 (2)	0.029 (2)	0.009 (2)
C14	0.0580 (19)	0.0370 (16)	0.0559 (19)	−0.0073 (15)	0.0220 (16)	−0.0062 (14)
C15	0.076 (3)	0.064 (3)	0.111 (4)	−0.004 (2)	0.053 (3)	−0.026 (2)
C16	0.097 (3)	0.060 (2)	0.044 (2)	−0.003 (2)	0.016 (2)	−0.0090 (16)
C17	0.0502 (17)	0.0444 (18)	0.0378 (16)	−0.0101 (14)	0.0075 (13)	0.0009 (13)
C18	0.053 (2)	0.061 (2)	0.054 (2)	−0.0102 (17)	0.0156 (16)	−0.0016 (16)
C19	0.062 (2)	0.079 (3)	0.068 (3)	−0.026 (2)	0.027 (2)	−0.005 (2)
C20	0.085 (3)	0.070 (3)	0.061 (2)	−0.038 (2)	0.023 (2)	−0.004 (2)
C21	0.084 (3)	0.051 (2)	0.054 (2)	−0.023 (2)	0.016 (2)	−0.0026 (16)
C22	0.064 (2)	0.0402 (17)	0.0408 (17)	−0.0136 (16)	0.0095 (16)	0.0018 (13)

Geometric parameters (Å, º)

C1—C2	1.375 (5)	C12—H12B	0.9600
C1—C6	1.377 (4)	C12—H12C	0.9600
C1—N1	1.449 (4)	C13—H13A	0.9600
C2—C3	1.380 (5)	C13—H13B	0.9600
C2—H2	0.9300	C13—H13C	0.9600
C3—C4	1.374 (5)	C14—N3	1.472 (4)
C3—H3	0.9300	C14—C16	1.504 (5)
C4—C5	1.369 (5)	C14—C15	1.539 (5)
C4—Cl1	1.751 (3)	C14—H14	0.9800
C5—C6	1.383 (5)	C15—H15A	0.9600
C5—H5	0.9300	C15—H15B	0.9600
C6—H6	0.9300	C15—H15C	0.9600
C7—N2	1.299 (4)	C16—H16A	0.9600
C7—N3	1.383 (4)	C16—H16B	0.9600
C7—N1	1.404 (4)	C16—H16C	0.9600
C8—C9	1.356 (5)	C17—C18	1.381 (5)
C8—N2	1.376 (4)	C17—C22	1.391 (5)
C8—C17	1.448 (5)	C18—C19	1.376 (5)
C9—O2	1.373 (4)	C18—H18	0.9300
C9—C10	1.423 (5)	C19—C20	1.392 (6)
C10—O1	1.218 (4)	C19—H19	0.9300
C10—N1	1.421 (4)	C20—C21	1.374 (6)
C11—N3	1.483 (4)	C20—H20	0.9300
C11—C13	1.515 (5)	C21—C22	1.380 (5)
C11—C12	1.528 (5)	C21—H21	0.9300
C11—H11	0.9800	C22—O2	1.379 (4)

C12—H12A	0.9600

C2—C1—C6	120.7 (3)	H13A—C13—H13C	109.5
C2—C1—N1	120.4 (3)	H13B—C13—H13C	109.5
C6—C1—N1	118.9 (3)	N3—C14—C16	109.5 (3)
C1—C2—C3	120.0 (3)	N3—C14—C15	117.4 (3)
C1—C2—H2	120.0	C16—C14—C15	110.9 (3)
C3—C2—H2	120.0	N3—C14—H14	106.1
C4—C3—C2	118.6 (3)	C16—C14—H14	106.1
C4—C3—H3	120.7	C15—C14—H14	106.1
C2—C3—H3	120.7	C14—C15—H15A	109.5
C5—C4—C3	121.9 (3)	C14—C15—H15B	109.5
C5—C4—Cl1	118.5 (3)	H15A—C15—H15B	109.5
C3—C4—Cl1	119.6 (3)	C14—C15—H15C	109.5
C4—C5—C6	119.1 (3)	H15A—C15—H15C	109.5
C4—C5—H5	120.4	H15B—C15—H15C	109.5
C6—C5—H5	120.4	C14—C16—H16A	109.5
C1—C6—C5	119.4 (3)	C14—C16—H16B	109.5
C1—C6—H6	120.3	H16A—C16—H16B	109.5
C5—C6—H6	120.3	C14—C16—H16C	109.5
N2—C7—N3	121.0 (3)	H16A—C16—H16C	109.5
N2—C7—N1	123.2 (3)	H16B—C16—H16C	109.5
N3—C7—N1	115.8 (3)	C18—C17—C22	119.6 (3)
C9—C8—N2	124.1 (3)	C18—C17—C8	136.0 (3)
C9—C8—C17	106.4 (3)	C22—C17—C8	104.3 (3)
N2—C8—C17	129.5 (3)	C19—C18—C17	118.3 (4)
C8—C9—O2	112.7 (3)	C19—C18—H18	120.9
C8—C9—C10	123.6 (3)	C17—C18—H18	120.9
O2—C9—C10	123.6 (3)	C18—C19—C20	121.1 (4)
O1—C10—N1	122.1 (3)	C18—C19—H19	119.5
O1—C10—C9	128.3 (3)	C20—C19—H19	119.5
N1—C10—C9	109.5 (3)	C21—C20—C19	121.7 (4)
N3—C11—C13	111.7 (3)	C21—C20—H20	119.2
N3—C11—C12	113.5 (4)	C19—C20—H20	119.2
C13—C11—C12	110.8 (3)	C20—C21—C22	116.5 (4)
N3—C11—H11	106.8	C20—C21—H21	121.8
C13—C11—H11	106.8	C22—C21—H21	121.8
C12—C11—H11	106.8	O2—C22—C21	125.0 (3)
C11—C12—H12A	109.5	O2—C22—C17	112.1 (3)
C11—C12—H12B	109.5	C21—C22—C17	122.9 (4)
H12A—C12—H12B	109.5	C7—N1—C10	124.2 (3)
C11—C12—H12C	109.5	C7—N1—C1	121.1 (2)
H12A—C12—H12C	109.5	C10—N1—C1	114.3 (3)
H12B—C12—H12C	109.5	C7—N2—C8	115.4 (3)
C11—C13—H13A	109.5	C7—N3—C14	119.4 (3)
C11—C13—H13B	109.5	C7—N3—C11	116.4 (2)
H13A—C13—H13B	109.5	C14—N3—C11	118.0 (2)
C11—C13—H13C	109.5	C9—O2—C22	104.5 (3)

C6—C1—C2—C3	4.1 (5)	N2—C7—N1—C10	−1.5 (5)
N1—C1—C2—C3	−177.7 (3)	N3—C7—N1—C10	179.4 (3)
C1—C2—C3—C4	−0.7 (5)	N2—C7—N1—C1	170.8 (3)
C2—C3—C4—C5	−2.7 (5)	N3—C7—N1—C1	−8.4 (4)
C2—C3—C4—Cl1	177.6 (3)	O1—C10—N1—C7	180.0 (3)
C3—C4—C5—C6	2.8 (5)	C9—C10—N1—C7	1.8 (4)
Cl1—C4—C5—C6	−177.5 (3)	O1—C10—N1—C1	7.2 (4)
C2—C1—C6—C5	−4.0 (5)	C9—C10—N1—C1	−171.0 (3)
N1—C1—C6—C5	177.8 (3)	C2—C1—N1—C7	105.9 (4)
C4—C5—C6—C1	0.6 (5)	C6—C1—N1—C7	−75.9 (4)
N2—C8—C9—O2	178.8 (3)	C2—C1—N1—C10	−81.1 (4)
C17—C8—C9—O2	1.2 (4)	C6—C1—N1—C10	97.1 (3)
N2—C8—C9—C10	−1.6 (5)	N3—C7—N2—C8	178.6 (3)
C17—C8—C9—C10	−179.3 (3)	N1—C7—N2—C8	−0.4 (4)
C8—C9—C10—O1	−178.4 (3)	C9—C8—N2—C7	2.0 (5)
O2—C9—C10—O1	1.1 (5)	C17—C8—N2—C7	179.0 (3)
C8—C9—C10—N1	−0.3 (4)	N2—C7—N3—C14	−42.8 (4)
O2—C9—C10—N1	179.2 (3)	N1—C7—N3—C14	136.3 (3)
C9—C8—C17—C18	177.2 (4)	N2—C7—N3—C11	109.0 (3)
N2—C8—C17—C18	−0.3 (6)	N1—C7—N3—C11	−71.9 (4)
C9—C8—C17—C22	−0.7 (3)	C16—C14—N3—C7	−66.1 (4)
N2—C8—C17—C22	−178.1 (3)	C15—C14—N3—C7	61.4 (4)
C22—C17—C18—C19	−1.0 (5)	C16—C14—N3—C11	142.5 (3)
C8—C17—C18—C19	−178.6 (4)	C15—C14—N3—C11	−89.9 (4)
C17—C18—C19—C20	1.9 (6)	C13—C11—N3—C7	140.8 (3)
C18—C19—C20—C21	−1.9 (7)	C12—C11—N3—C7	−93.0 (4)
C19—C20—C21—C22	0.8 (6)	C13—C11—N3—C14	−67.0 (4)
C20—C21—C22—O2	178.2 (3)	C12—C11—N3—C14	59.2 (4)
C20—C21—C22—C17	0.1 (5)	C8—C9—O2—C22	−1.2 (3)
C18—C17—C22—O2	−178.3 (3)	C10—C9—O2—C22	179.3 (3)
C8—C17—C22—O2	0.0 (3)	C21—C22—O2—C9	−177.5 (3)
C18—C17—C22—C21	0.0 (5)	C17—C22—O2—C9	0.7 (3)
C8—C17—C22—C21	178.3 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15*A*···N2	0.96	2.44	2.946 (5)	113