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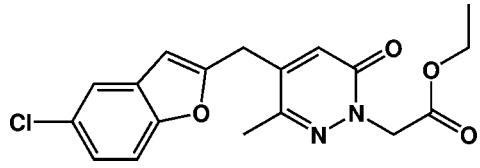

Crystal structure of ethyl 2-{4-[(5-chloro-1-benzofuran-2-yl)methyl]-3-methyl-6-oxo-1,6-dihydropyridazin-1-yl}acetate

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In the title compound, $C_{18}H_{17}ClN_2O_4$, the dihedral angle between the benzofuran ring system [maximum deviation 0.014 (2) Å] and the oxopyradizine ring is 73.33 (8)°. The structure is characterized by disorder of the ethyl group, which is split into two parts, with a major component of 0.57 (3), and the acetate carbonyl O atom, which is statistically disordered. In the crystal, the molecules are linked by C—H···O interactions, forming a three-dimensional network.

Keywords: crystal structure; pyridazinone derivative; hydrogen bonding.

CCDC reference: 1056731

1. Related literature

For pharmacological activities of pyridazinones, *e.g.* antimicrobial, see: Boukharsa *et al.* (2014); Nagle *et al.* (2014); El-Hashash *et al.* (2014); Tiryaki *et al.* (2013); Csókás *et al.* (2013); Asif *et al.* (2014); Garkani-Nejad & Poshteh-Shirani (2013). For biological activities of pyridazinone derivatives and their applications, *e.g.* as insecticides and herbicides, see: Cao *et al.* (2003); Jamet & Piedallu (1975). For pyridazin-3(2*H*)-one derivatives, see: Taoufik *et al.* (1984); Benchat *et al.* (1998); Abourichaa *et al.* (2003).

2. Experimental

2.1. Crystal data

$C_{18}H_{17}ClN_2O_4$
M_r = 360.79
Orthorhombic, $P2_12_12_1$
a = 7.9792 (2) Å
b = 8.7460 (2) Å
c = 25.2064 (6) Å
V = 1759.06 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 296 K
0.37 × 0.34 × 0.29 mm

2.2. Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.589, T_{max} = 0.746
12689 measured reflections
4925 independent reflections
3350 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.114
S = 1.02
4925 reflections
255 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}
Absolute structure: Flack & Bernardinelli (2000), 2104 Friedel pairs
Absolute structure parameter: 0.02 (7)

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···O3B^{i}	0.93	2.37	3.291 (19)	170
C15—H15B···O2^{ii}	0.97	2.34	3.278 (3)	161
C18A—H18A···O2^{iii}	0.96	2.41	3.310 (10)	156

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: TK5363).

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supporting information

Acta Cryst. (2015). E**71**, o291–o292 [https://doi.org/10.1107/S2056989015006301]

Crystal structure of ethyl 2-{4-[(5-chloro-1-benzofuran-2-yl)methyl]-3-methyl-6-oxo-1,6-dihydropyridazin-1-yl}acetate

Youness Boukharsa, Lahcen El Ammari, Jamal Taoufik, Mohamed Saadi and M'hammed Ansar

S1. Comment

During recent years, pyridazinones have been a subject of numerous recent studies (Boukharsa *et al.*, 2014) owing to their wide spectrum of pharmacological activities such as antimicrobial (Nagle *et al.*, 2014), anti-fungal (El-Hashash *et al.*, 2014), analgesic & anti-inflammatory (Tiryaki *et al.*, 2013), anticancer (Csókás *et al.*, 2013), anti-tubercular (Asif *et al.*, 2014) and anti-hypertensive activities (Garkani-Nejad & Poshteh-Shirani, 2013). It has also been reported that pyridazinone derivative have remarkable insecticidal (Cao *et al.*, 2003) and herbicidal activities (Jamet & Piedallu, 1975). In continuation of this line of research (Taoufik *et al.*, 1984; Benchat *et al.*, 1998; Abourichaa *et al.*, 2003), we have developed a new pyridazin-3(2*H*)-one derivative. It will be subjected to further pharmacological investigations, especially tests of anticancer activity. Compound (I) is stable at room temperature, and its structure has been determined by NMR (^{1}H and ^{13} C). In this paper we wish to report the crystal structure determination of the title compound possessing the biologically active pyridazinone ring.

The molecule of the title compound is build up from 5-chlorobenzofuran-2-yl linked, *via* –CH_2– group, to six-membered heterocyclic ring which is related to acetate group as shown in Fig. 1. The benzofuran system is virtually planar with the largest deviation from the mean plane being -0.014 (2) Å at C4, and makes dihedral angle of 73.33 (8)° with the mean plane through the oxopyridazin (C10–C13,N1,N2) ring. Non classical C—H···O hydrogen bonds link the molecules into a three-dimensional network.

S2. Experimental

To a solution of 5-((5-chlorobenzofuran-2-yl)methyl)-6-methylpyridazin-3(2*H*)-one (0.5 g, 1.82 mmol) dissolved in tetrahydrofuran (15 ml) was added ethyl 2-bromoacetate (0.30 ml, 2.73 mmol), potassium carbonate (0.5 g, 3.64 mmol) and a catalytic amount of tetra-n-butylammonium bromide (0.05 g, 0.15 mmol). The mixture was stirred at room temperature for 6 h, and monitored by thin layer chromatography. The compound was removed by filtration and the filtrate concentrated under vacuum. The solid obtained was crystallized from ethanol to afford colourless crystals (Yield = 77%; M.pt = 136.9 °C).

S3. Refinement

The H atoms were located in a difference map and treated as riding with C—H = 0.93 Å (aromatic), C—H = 0.97 Å (methylene) and C—H = 0.96 Å (methyl), and with U_{iso}(H) = 1.2 U_{eq} (aromatic and methylene) and U_{iso}(H) = 1.5 U_{eq} for methyl. This structure is characterized by a partial disorder at the acetate group, with the ethyl group split into two parts. The major component had a site occupancy factor = 0.57 (3). The carbonyl-O3 was statistically disordered. Owing to poor agreement, the (0 0 2) reflection was omitted from the final cycles of refinement.

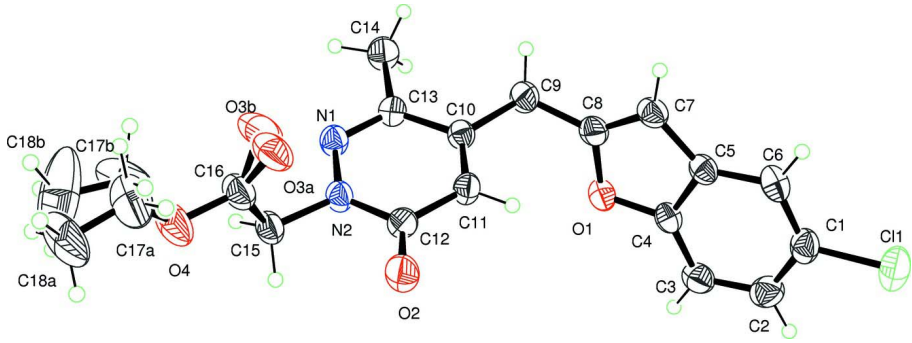

Figure 1

Molecular structure of the title compound with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small circles.

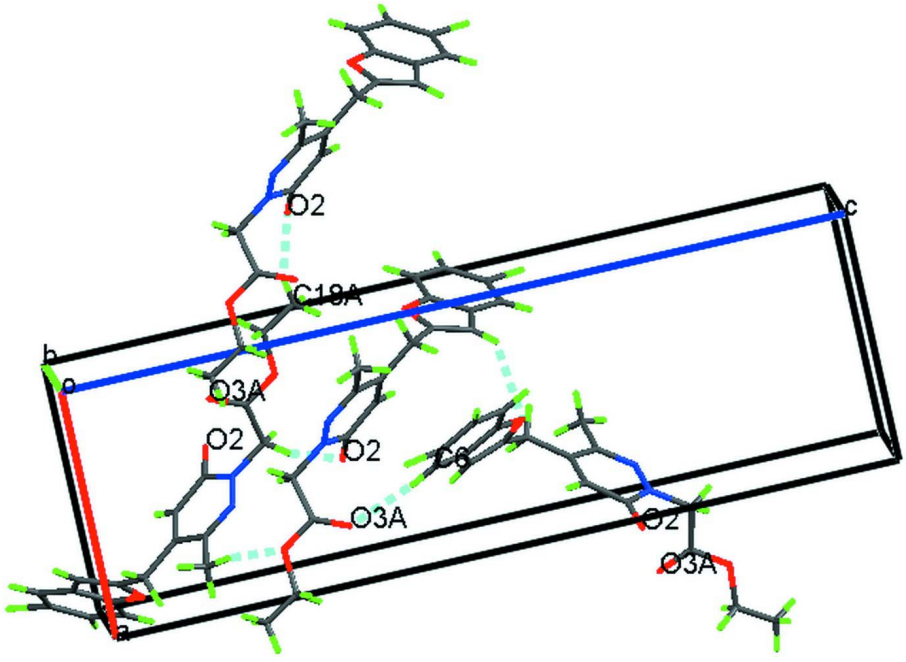

Figure 2

Crystal packing in the structure of the title compound, showing molecules linked by C—H···O hydrogen bonds (dashed lines).

Ethyl 2-{4-[(5-chloro-1-benzofuran-2-yl)methyl]-3-methyl-6-oxo-1,6-dihydropyridazin-1-yl}acetate

Crystal data

$C_{18}H_{17}ClN_2O_4$
M_r = 360.79
Orthorhombic, $P2_12_12_1$
Hall symbol: p 2ac 2ab
a = 7.9792 (2) Å
b = 8.7460 (2) Å
c = 25.2064 (6) Å
V = 1759.06 (7) Å^3
Z = 4

$F(000)$ = 752
D_x = 1.362 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4925 reflections
θ = 2.5–29.6°
μ = 0.24 mm^{-1}
T = 296 K
Block, colourless
0.37 × 0.34 × 0.29 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.589, T_{max} = 0.746
12689 measured reflections
4925 independent reflections
3350 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 29.6°, θ_{min} = 2.5°
h = −11→6
k = −12→11
l = −35→34

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.114
S = 1.02
4925 reflections
255 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0511P)^2 + 0.0996P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.043
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}
Absolute structure: Flack & Bernardinelli (2000), 2104 Friedel pairs
Absolute structure parameter: 0.02 (7)

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	0.0331 (3)	0.7077 (3)	0.55647 (8)	0.0497 (5)	
C2	−0.0495 (3)	0.7389 (3)	0.50905 (9)	0.0551 (6)	
H2	−0.1006	0.8335	0.5042	0.066*	
C3	−0.0561 (3)	0.6314 (3)	0.46924 (8)	0.0500 (5)	
H3	−0.1101	0.6507	0.4372	0.060*	
C4	0.0215 (2)	0.4935 (2)	0.47935 (7)	0.0408 (4)	
C5	0.1023 (2)	0.4581 (2)	0.52669 (7)	0.0401 (5)	
C6	0.1087 (3)	0.5691 (3)	0.56674 (8)	0.0493 (6)	
H6	0.1618	0.5500	0.5989	0.059*	
C7	0.1597 (3)	0.3032 (3)	0.52045 (8)	0.0448 (5)	
H7	0.2188	0.2460	0.5453	0.054*	
C8	0.1118 (3)	0.2568 (3)	0.47190 (8)	0.0431 (5)	
C9	0.1316 (3)	0.1120 (3)	0.44154 (8)	0.0472 (5)	
H9A	0.0220	0.0785	0.4297	0.057*	
H9B	0.1755	0.0342	0.4652	0.057*	

C10	0.2463 (2)	0.1236 (2)	0.39358 (7)	0.0368 (4)	
C11	0.3432 (2)	0.2461 (2)	0.38377 (7)	0.0414 (4)	
H11	0.3383	0.3299	0.4064	0.050*	
C12	0.4547 (3)	0.2499 (2)	0.33859 (8)	0.0409 (4)	
C13	0.2541 (2)	−0.0037 (3)	0.35783 (7)	0.0384 (4)	
C14	0.1523 (3)	−0.1455 (3)	0.36636 (9)	0.0514 (5)	
H14A	0.1751	−0.2173	0.3385	0.077*	
H14B	0.0353	−0.1198	0.3662	0.077*	
H14C	0.1812	−0.1902	0.3999	0.077*	
C15	0.5492 (3)	0.1158 (3)	0.25914 (8)	0.0460 (5)	
H15A	0.5611	0.2173	0.2441	0.055*	
H15B	0.4950	0.0513	0.2329	0.055*	
C16	0.7196 (3)	0.0523 (3)	0.27179 (9)	0.0570 (6)	
C17A	0.9885 (15)	0.004 (2)	0.2313 (4)	0.090 (4)	0.57 (3)
H17A	1.0439	0.0692	0.2571	0.108*	0.57 (3)
H17B	0.9939	−0.0998	0.2446	0.108*	0.57 (3)
C18A	1.0731 (14)	0.0109 (18)	0.1866 (4)	0.115 (5)	0.57 (3)
H18A	1.1866	−0.0209	0.1927	0.173*	0.57 (3)
H18B	1.0723	0.1140	0.1735	0.173*	0.57 (3)
H18C	1.0220	−0.0555	0.1609	0.173*	0.57 (3)
C17B	0.967 (2)	−0.045 (3)	0.2318 (8)	0.136 (9)	0.43 (3)
H17C	1.0491	0.0111	0.2524	0.164*	0.43 (3)
H17D	0.9406	−0.1378	0.2511	0.164*	0.43 (3)
C18B	1.027 (3)	−0.078 (5)	0.1915 (11)	0.201 (15)	0.43 (3)
H18D	1.1232	−0.1419	0.1977	0.302*	0.43 (3)
H18E	1.0608	0.0124	0.1729	0.302*	0.43 (3)
H18F	0.9469	−0.1334	0.1705	0.302*	0.43 (3)
N1	0.3493 (2)	−0.0030 (2)	0.31573 (6)	0.0420 (4)	
N2	0.4446 (2)	0.12399 (19)	0.30664 (6)	0.0407 (4)	
O1	0.02722 (17)	0.37131 (17)	0.44539 (5)	0.0441 (3)	
O2	0.5521 (2)	0.35450 (19)	0.32838 (6)	0.0604 (4)	
O3A	0.776 (2)	0.037 (5)	0.3148 (7)	0.069 (5)	0.50 (10)
O3B	0.756 (4)	−0.019 (7)	0.3125 (11)	0.088 (6)	0.50 (10)
O4	0.8114 (2)	0.0497 (3)	0.22828 (6)	0.0776 (7)	
Cl1	0.04000 (9)	0.85141 (8)	0.60423 (3)	0.0730 (2)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0478 (12)	0.0520 (13)	0.0493 (11)	−0.0015 (11)	0.0142 (10)	−0.0084 (11)
C2	0.0546 (14)	0.0482 (12)	0.0626 (13)	0.0075 (12)	0.0102 (11)	0.0050 (12)
C3	0.0488 (12)	0.0569 (13)	0.0443 (10)	0.0067 (11)	0.0026 (9)	0.0085 (11)
C4	0.0382 (10)	0.0484 (11)	0.0358 (9)	−0.0006 (9)	0.0078 (8)	−0.0005 (9)
C5	0.0345 (10)	0.0498 (12)	0.0359 (9)	0.0013 (8)	0.0070 (8)	0.0022 (10)
C6	0.0447 (12)	0.0665 (15)	0.0367 (10)	−0.0003 (10)	0.0053 (9)	−0.0045 (11)
C7	0.0416 (11)	0.0528 (13)	0.0401 (10)	0.0069 (9)	0.0050 (9)	0.0063 (10)
C8	0.0390 (11)	0.0473 (12)	0.0430 (10)	0.0028 (9)	0.0124 (9)	0.0046 (10)
C9	0.0465 (12)	0.0468 (12)	0.0483 (11)	−0.0017 (10)	0.0151 (9)	−0.0004 (11)

C10	0.0324 (9)	0.0403 (11)	0.0377 (9)	0.0021 (8)	0.0025 (7)	−0.0010 (9)
C11	0.0407 (11)	0.0402 (11)	0.0433 (10)	−0.0007 (9)	0.0069 (8)	−0.0071 (9)
C12	0.0364 (10)	0.0396 (10)	0.0466 (10)	−0.0023 (9)	0.0049 (8)	−0.0003 (9)
C13	0.0342 (9)	0.0410 (11)	0.0400 (9)	−0.0008 (8)	−0.0001 (8)	−0.0031 (9)
C14	0.0514 (13)	0.0480 (13)	0.0549 (12)	−0.0116 (11)	0.0066 (10)	−0.0053 (12)
C15	0.0453 (11)	0.0537 (13)	0.0390 (10)	0.0022 (11)	0.0098 (9)	−0.0005 (10)
C16	0.0521 (13)	0.0725 (18)	0.0463 (12)	0.0110 (12)	0.0144 (11)	0.0093 (13)
C17A	0.061 (5)	0.144 (10)	0.064 (4)	0.038 (5)	−0.005 (4)	0.003 (6)
C18A	0.061 (5)	0.197 (12)	0.088 (6)	0.058 (6)	0.045 (4)	0.051 (8)
C17B	0.068 (7)	0.191 (18)	0.150 (13)	0.082 (9)	0.079 (8)	0.109 (12)
C18B	0.098 (14)	0.31 (4)	0.195 (19)	0.098 (18)	−0.032 (12)	−0.15 (2)
N1	0.0421 (9)	0.0420 (10)	0.0420 (9)	−0.0047 (7)	0.0043 (7)	−0.0046 (8)
N2	0.0385 (9)	0.0433 (9)	0.0403 (8)	−0.0028 (8)	0.0092 (7)	−0.0037 (8)
O1	0.0458 (8)	0.0520 (9)	0.0345 (6)	0.0025 (7)	0.0015 (6)	−0.0032 (7)
O2	0.0626 (10)	0.0545 (10)	0.0640 (9)	−0.0194 (9)	0.0233 (8)	−0.0068 (9)
O3A	0.063 (4)	0.096 (10)	0.047 (4)	0.021 (5)	0.006 (3)	0.022 (5)
O3B	0.086 (7)	0.110 (15)	0.069 (5)	0.038 (8)	0.029 (4)	0.046 (7)
O4	0.0519 (10)	0.1259 (19)	0.0549 (9)	0.0329 (11)	0.0193 (8)	0.0216 (11)
Cl1	0.0791 (5)	0.0674 (4)	0.0725 (4)	−0.0034 (4)	0.0133 (3)	−0.0271 (3)

Geometric parameters (Å, º)

C1—C6	1.378 (3)	C13—C14	1.498 (3)
C1—C2	1.392 (3)	C14—H14A	0.9600
C1—Cl1	1.742 (2)	C14—H14B	0.9600
C2—C3	1.376 (3)	C14—H14C	0.9600
C2—H2	0.9300	C15—N2	1.461 (2)
C3—C4	1.380 (3)	C15—C16	1.504 (3)
C3—H3	0.9300	C15—H15A	0.9700
C4—O1	1.370 (2)	C15—H15B	0.9700
C4—C5	1.391 (3)	C16—O3A	1.182 (17)
C5—C6	1.401 (3)	C16—O3B	1.234 (17)
C5—C7	1.439 (3)	C16—O4	1.319 (2)
C6—H6	0.9300	C17A—C18A	1.316 (15)
C7—C8	1.345 (3)	C17A—O4	1.470 (12)
C7—H7	0.9300	C17A—H17A	0.9700
C8—O1	1.380 (3)	C17A—H17B	0.9700
C8—C9	1.488 (3)	C18A—H18A	0.9600
C9—C10	1.520 (3)	C18A—H18B	0.9600
C9—H9A	0.9700	C18A—H18C	0.9600
C9—H9B	0.9700	C17B—C18B	1.16 (3)
C10—C11	1.344 (3)	C17B—O4	1.493 (18)
C10—C13	1.434 (3)	C17B—H17C	0.9700
C11—C12	1.446 (3)	C17B—H17D	0.9700
C11—H11	0.9300	C18B—H18D	0.9600
C12—O2	1.228 (2)	C18B—H18E	0.9600
C12—N2	1.367 (3)	C18B—H18F	0.9600
C13—N1	1.305 (2)	N1—N2	1.365 (2)

C6—C1—C2	122.8 (2)	H14A—C14—H14C	109.5
C6—C1—Cl1	119.41 (17)	H14B—C14—H14C	109.5
C2—C1—Cl1	117.82 (18)	N2—C15—C16	111.14 (17)
C3—C2—C1	120.7 (2)	N2—C15—H15A	109.4
C3—C2—H2	119.7	C16—C15—H15A	109.4
C1—C2—H2	119.7	N2—C15—H15B	109.4
C2—C3—C4	116.43 (19)	C16—C15—H15B	109.4
C2—C3—H3	121.8	H15A—C15—H15B	108.0
C4—C3—H3	121.8	O3A—C16—O3B	24.8 (15)
O1—C4—C3	125.54 (18)	O3A—C16—O4	123.2 (9)
O1—C4—C5	110.30 (18)	O3B—C16—O4	123.6 (10)
C3—C4—C5	124.13 (19)	O3A—C16—C15	125.6 (9)
C4—C5—C6	118.7 (2)	O3B—C16—C15	124.9 (11)
C4—C5—C7	105.27 (18)	O4—C16—C15	109.41 (19)
C6—C5—C7	136.0 (2)	C18A—C17A—O4	115.8 (9)
C1—C6—C5	117.23 (19)	C18A—C17A—H17A	108.3
C1—C6—H6	121.4	O4—C17A—H17A	108.3
C5—C6—H6	121.4	C18A—C17A—H17B	108.3
C8—C7—C5	107.06 (19)	O4—C17A—H17B	108.3
C8—C7—H7	126.5	H17A—C17A—H17B	107.4
C5—C7—H7	126.5	C17A—C18A—H18A	109.5
C7—C8—O1	111.11 (19)	C17A—C18A—H18B	109.5
C7—C8—C9	134.0 (2)	H18A—C18A—H18B	109.5
O1—C8—C9	114.88 (17)	C17A—C18A—H18C	109.5
C8—C9—C10	114.63 (18)	H18A—C18A—H18C	109.5
C8—C9—H9A	108.6	H18B—C18A—H18C	109.5
C10—C9—H9A	108.6	C18B—C17B—O4	115.6 (19)
C8—C9—H9B	108.6	C18B—C17B—H17C	108.3
C10—C9—H9B	108.6	O4—C17B—H17C	108.4
H9A—C9—H9B	107.6	C18B—C17B—H17D	108.5
C11—C10—C13	118.60 (17)	O4—C17B—H17D	108.4
C11—C10—C9	123.06 (18)	H17C—C17B—H17D	107.4
C13—C10—C9	118.33 (18)	C17B—C18B—H18D	109.4
C10—C11—C12	121.13 (18)	C17B—C18B—H18E	109.6
C10—C11—H11	119.4	H18D—C18B—H18E	109.5
C12—C11—H11	119.4	C17B—C18B—H18F	109.4
O2—C12—N2	120.95 (17)	H18D—C18B—H18F	109.5
O2—C12—C11	124.88 (19)	H18E—C18B—H18F	109.5
N2—C12—C11	114.17 (17)	C13—N1—N2	117.70 (16)
N1—C13—C10	122.17 (19)	N1—N2—C12	126.10 (15)
N1—C13—C14	115.89 (18)	N1—N2—C15	114.57 (16)
C10—C13—C14	121.94 (17)	C12—N2—C15	119.25 (16)
C13—C14—H14A	109.5	C4—O1—C8	106.25 (15)
C13—C14—H14B	109.5	C16—O4—C17A	119.7 (5)
H14A—C14—H14B	109.5	C16—O4—C17B	114.9 (7)
C13—C14—H14C	109.5	C17A—O4—C17B	17.9 (15)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···O3*B*^{i}	0.93	2.37	3.291 (19)	170
C15—H15*B*···O2^{ii}	0.97	2.34	3.278 (3)	161
C18*A*—H18*A*···O2^{iii}	0.96	2.41	3.310 (10)	156

Symmetry codes: (i) *x*−1/2, −*y*+1/2, −*z*+1; (ii) −*x*+1, *y*−1/2, −*z*+1/2; (iii) −*x*+2, *y*−1/2, −*z*+1/2.