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3,3′-(1,4-Phenylene)bis[2-(propylamino)-benzofuro[3,2-*d*]pyrimidin-4(3*H*)-one] ethanol disolvate

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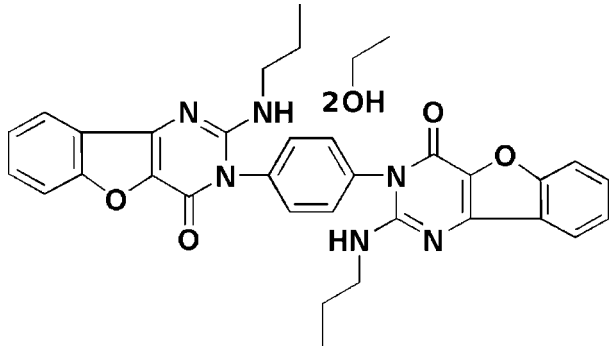
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.054; wR factor = 0.151; data-to-parameter ratio = 11.4.

The title compound, $C_{32}H_{28}N_6O_4\cdot 2C_2H_5OH$, consists of two 2-(propylamino)benzofuro[3,2-*d*]pyrimidin-4(3*H*)-one units connected, *via* one of the pyrimidine N atoms, to a bridging benzene ring in the 1,4 positions. Two ethanol solvent molecules are also present. The main molecule lies on a center of symmetry located at the center of the benzene ring. The fused-ring system of the benzofuro[3,2-*d*]pyrimidine moiety is nearly planar (r.m.s. deviation = 0.016 Å) and forms a dihedral angle of 78.21 (7)° with the central benzene ring. The crystal structure features O—H···O and N—H···O interactions. The C atoms of the propylamino side chain in the main molecule and the ethyl group in the solvent molecule are disordered over two positions, with site-occupancy factors 0.34:0.66 and 0.42:0.58, respectively.

Related literature

The title compound may be used as a precursor for obtaining bioactive molecules with antitumor activity, see: Bellarosa *et al.* (1996). For the biological activity of benzofuropyrimidine derivatives, see: Moneam *et al.* (2004); Bodke & Sangapure (2003). For the crystal structures of other fused pyrimidinone derivatives, see: Hu *et al.* (2005, 2006, 2007, 2008).



Experimental

Crystal data

$C_{32}H_{28}N_6O_4\cdot 2C_2H_6O$
M_r = 652.74
Monoclinic, $P2_1/n$
a = 10.1933 (12) Å
b = 13.6224 (16) Å
c = 12.5249 (15) Å
β = 105.409 (2)°
V = 1676.7 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 K
0.14 × 0.12 × 0.10 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.988, T_{max} = 0.991
10883 measured reflections
2941 independent reflections
2327 reflections with $I > 2\sigma(I)$
R_{int} = 0.060

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.151
S = 1.03
2941 reflections
259 parameters
60 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3a···O3	0.86	2.22	2.996 (3)	150
O3—H3b···O1^{i}	0.82	2.12	2.903 (3)	159

Symmetry code: (i) $-x+1, -y, -z+1$.

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).

The authors are grateful to Dr X. G. Meng (Key Laboratory of Pesticides & Chemical Biology of the Ministry of Education, Central China Normal University, Wuhan, Hubei, China) for the data collection and analysis. This work was supported by the Natural Science Foundation of Hubei Provincial Department of Science and Technology (No. 2011CDB08301) and the Science Research Project of Hubei University of Medicine (Nos. 2011CXX03 and No. 2009QDJ15).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LR2054).

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supplementary materials

Acta Cryst. (2012). E**68**, o1282–o1283 [doi:10.1107/S160053681201375X]

3,3′-(1,4-Phenylene)bis[2-(propylamino)benzofuro[3,2-*d*]pyrimidin-4(3*H*)-one] ethanol disolvate

Li Li, Yong-Nian Qu, Jian Gong and Yang-Gen Hu

Comment

As a part of our ongoing work in the preparation of derivatives of heterocyclic compounds (Hu *et al.*, 2005, 2006, 2007, 2008), we have synthesized and structurally characterized the title compound (Fig. 1). Here we wish to report an X-ray crystal structure of it (Fig. 1). In the molecule, the fused rings system of the benzo[4,5]furo[3,2-*d*]pyrimidine system are nearly coplanar (r.m.s. deviation= 0.016 A°), forming a dihedral angle of 78.21 (7)° with the (C1/C2/C3/C1a/C2a/C3a) phenyl ring . The crystal structure is stabilize by O—H···O and N—H···O hydrogen bonds. The C atoms of the propyl-amino side chain in molecule and the ethyl in solvent molecule are disordered over two positions, with site occupancy factors 0.34/0.66 and 0.42/58 for the C atoms of the propyl and the ethyl, respectively.

Experimental

The compound was synthesized according to the procedures previously described in the literature (Hu *et al.*, 2005, 2006, 2007, 2008).

Refinement

All H-atoms were positioned with idealized geometry and refined isotropic (U_{iso}(H)= 1.5U_{eq}(C)for methyl H atoms and U_{iso}(H) =1.2U_{eq}(C) for all other H atoms) using a riding model with C—H = 0.93°, 0.97° and 0.96 Å, O—H = 0.82°, N—H = 0.86°.

Computing details

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

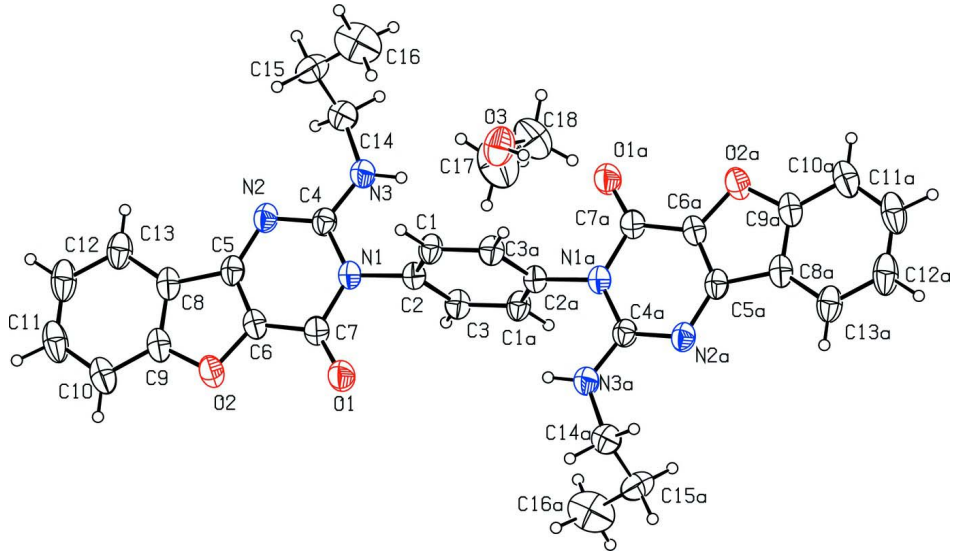

Figure 1

The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

3,3′-(1,4-Phenylene)bis[2-(propylamino)benzofuro[3,2-*d*]pyrimidin- 4(3*H*)-one] ethanol disolvate

Crystal data

$C_{32}H_{28}N_6O_4·2C_2H_6O$
M_r = 652.74
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 10.1933 (12) Å
b = 13.6224 (16) Å
c = 12.5249 (15) Å
β = 105.409 (2)°
V = 1676.7 (3) Å^3
Z = 2
$F(000)$ = 692
D_x = 1.293 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3984 reflections
θ = 2.3–26.6°
μ = 0.09 mm^{-1}
T = 298 K
Block, colorless
0.14 × 0.12 × 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} = 0.988, T_{max} = 0.991
10883 measured reflections
2941 independent reflections
2327 reflections with $I > 2\sigma(I)$
R_{int} = 0.060
θ_{max} = 25.0°, θ_{min} = 2.3°
h = −12→12
k = −13→16
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.151
S = 1.03
2941 reflections
259 parameters
60 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

$w = 1/[\sigma^2(F_o^2) + (0.0753P)^2 + 0.3428P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.6148 (2)	0.02496 (15)	0.58223 (16)	0.0567 (5)	
H1	0.6919	0.0422	0.6376	0.068*	
C2	0.53256 (19)	0.09654 (14)	0.52147 (15)	0.0506 (5)	
C3	0.4179 (2)	0.07207 (15)	0.43955 (16)	0.0561 (5)	
H3	0.3628	0.1210	0.3991	0.067*	
C4	0.6653 (2)	0.24409 (15)	0.50513 (16)	0.0538 (5)	
C5	0.6309 (2)	0.38471 (15)	0.58744 (16)	0.0546 (5)	
C6	0.5310 (2)	0.34514 (15)	0.62721 (17)	0.0594 (6)	
C7	0.4899 (2)	0.24663 (16)	0.60962 (17)	0.0588 (5)	
C8	0.6399 (2)	0.48678 (14)	0.62188 (17)	0.0587 (6)	
C9	0.5417 (3)	0.49804 (15)	0.67922 (18)	0.0654 (6)	
C10	0.5178 (3)	0.58535 (18)	0.7266 (2)	0.0794 (7)	
H10	0.4514	0.5909	0.7647	0.095*	
C11	0.5975 (3)	0.66348 (18)	0.7143 (2)	0.0870 (9)	
H11	0.5855	0.7236	0.7456	0.104*	
C12	0.6954 (3)	0.65482 (17)	0.6563 (2)	0.0861 (9)	
H12	0.7473	0.7094	0.6494	0.103*	
C13	0.7177 (3)	0.56759 (16)	0.6088 (2)	0.0727 (7)	
H13	0.7827	0.5627	0.5692	0.087*	
C14	0.8284 (3)	0.2270 (2)	0.3940 (3)	0.0960 (9)	
H14A	0.8253	0.1882	0.3285	0.115*	0.58
H14B	0.8023	0.2933	0.3688	0.115*	0.58
H14C	0.8351	0.2980	0.3990	0.115*	0.42
H14D	0.8145	0.2068	0.3176	0.115*	0.42
C15	0.9688 (6)	0.2310 (5)	0.4575 (7)	0.118 (2)	0.58
H15A	0.9764	0.2644	0.5272	0.141*	0.58
H15B	1.0223	0.2667	0.4168	0.141*	0.58
C16	1.0198 (10)	0.1280 (6)	0.4782 (7)	0.138 (3)	0.58
H16A	0.9695	0.0943	0.5219	0.207*	0.58
H16B	1.1146	0.1289	0.5172	0.207*	0.58
H16C	1.0081	0.0946	0.4088	0.207*	0.58
C15′	0.9540 (9)	0.1753 (13)	0.4727 (13)	0.161 (6)	0.42
H15C	0.9605	0.1952	0.5483	0.194*	0.42

H15D	0.9395	0.1049	0.4682	0.194*	0.42
C16′	1.0849 (9)	0.1976 (10)	0.4471 (10)	0.149 (4)	0.42
H16D	1.1045	0.1473	0.3999	0.223*	0.42
H16E	1.1566	0.1999	0.5147	0.223*	0.42
H16F	1.0784	0.2599	0.4103	0.223*	0.42
C17	0.5680 (9)	0.0856 (5)	0.1674 (7)	0.148 (3)	0.66
H17A	0.5009	0.1024	0.2055	0.223*	0.66
H17B	0.5254	0.0807	0.0894	0.223*	0.66
H17C	0.6368	0.1356	0.1803	0.223*	0.66
C18	0.6292 (9)	−0.0070 (5)	0.2079 (5)	0.118 (2)	0.66
H18A	0.5617	−0.0588	0.1878	0.142*	0.66
H18B	0.7020	−0.0216	0.1737	0.142*	0.66
C17′	0.6268 (14)	0.0358 (14)	0.1313 (9)	0.137 (4)	0.34
H17D	0.7050	0.0778	0.1528	0.205*	0.34
H17E	0.5587	0.0665	0.0728	0.205*	0.34
H17F	0.6527	−0.0258	0.1058	0.205*	0.34
C18′	0.5711 (10)	0.0189 (12)	0.2276 (7)	0.099 (3)	0.34
H18C	0.5239	0.0772	0.2420	0.118*	0.34
H18D	0.5064	−0.0349	0.2119	0.118*	0.34
N1	0.56533 (17)	0.19870 (11)	0.54545 (13)	0.0526 (4)	
N2	0.70225 (18)	0.33593 (12)	0.52685 (15)	0.0586 (5)	
N3	0.7232 (2)	0.18964 (13)	0.44097 (17)	0.0680 (5)	
H3A	0.6966	0.1299	0.4271	0.082*	
O1	0.40323 (19)	0.20284 (12)	0.64207 (15)	0.0807 (5)	
O2	0.47273 (17)	0.41186 (11)	0.68384 (13)	0.0729 (5)	
O3	0.6821 (2)	−0.00452 (14)	0.32441 (15)	0.0915 (6)	
H3B	0.6693	−0.0577	0.3506	0.137*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0582 (12)	0.0497 (12)	0.0530 (11)	−0.0030 (9)	−0.0011 (9)	−0.0018 (9)
C2	0.0579 (12)	0.0437 (11)	0.0488 (10)	−0.0026 (9)	0.0118 (9)	−0.0019 (8)
C3	0.0608 (12)	0.0466 (12)	0.0537 (11)	0.0037 (9)	0.0028 (9)	0.0055 (9)
C4	0.0551 (12)	0.0461 (11)	0.0563 (11)	−0.0006 (9)	0.0076 (9)	0.0007 (9)
C5	0.0603 (12)	0.0448 (11)	0.0500 (10)	−0.0001 (9)	−0.0006 (9)	0.0004 (9)
C6	0.0698 (13)	0.0472 (12)	0.0582 (12)	0.0014 (10)	0.0115 (10)	−0.0089 (9)
C7	0.0677 (13)	0.0522 (12)	0.0563 (12)	−0.0050 (11)	0.0160 (10)	−0.0041 (10)
C8	0.0683 (13)	0.0435 (11)	0.0517 (11)	0.0035 (10)	−0.0061 (10)	−0.0004 (9)
C9	0.0775 (15)	0.0475 (13)	0.0591 (12)	0.0056 (11)	−0.0028 (11)	−0.0069 (10)
C10	0.0969 (19)	0.0583 (15)	0.0710 (15)	0.0152 (13)	0.0012 (13)	−0.0132 (12)
C11	0.115 (2)	0.0478 (14)	0.0770 (17)	0.0193 (15)	−0.0122 (16)	−0.0084 (12)
C12	0.111 (2)	0.0410 (13)	0.0850 (17)	0.0000 (13)	−0.0106 (16)	0.0040 (12)
C13	0.0867 (17)	0.0468 (13)	0.0709 (14)	−0.0030 (11)	−0.0030 (12)	0.0050 (10)
C14	0.094 (2)	0.0741 (18)	0.136 (3)	−0.0151 (16)	0.059 (2)	−0.0216 (17)
C15	0.082 (4)	0.139 (6)	0.149 (5)	−0.045 (4)	0.060 (4)	−0.051 (5)
C16	0.142 (6)	0.163 (7)	0.107 (4)	0.039 (5)	0.029 (4)	0.018 (4)
C15′	0.142 (9)	0.174 (10)	0.181 (9)	−0.029 (8)	0.065 (8)	0.033 (8)
C16′	0.098 (6)	0.193 (9)	0.156 (7)	0.000 (6)	0.037 (5)	0.007 (7)
C17	0.183 (6)	0.123 (5)	0.118 (4)	0.041 (4)	0.001 (4)	0.004 (4)

C18	0.155 (6)	0.110 (4)	0.094 (4)	0.021 (4)	0.042 (4)	−0.005 (3)
C17′	0.151 (8)	0.157 (9)	0.107 (7)	0.029 (7)	0.042 (6)	0.029 (7)
C18′	0.095 (6)	0.121 (8)	0.083 (6)	0.002 (6)	0.030 (5)	0.000 (6)
N1	0.0602 (10)	0.0416 (9)	0.0541 (9)	−0.0036 (7)	0.0120 (8)	−0.0030 (7)
N2	0.0621 (10)	0.0441 (10)	0.0661 (11)	−0.0044 (8)	0.0110 (8)	−0.0015 (8)
N3	0.0744 (12)	0.0507 (10)	0.0860 (13)	−0.0094 (9)	0.0339 (10)	−0.0097 (9)
O1	0.0978 (13)	0.0648 (11)	0.0927 (12)	−0.0184 (9)	0.0484 (11)	−0.0170 (9)
O2	0.0882 (11)	0.0563 (10)	0.0750 (10)	−0.0013 (8)	0.0233 (9)	−0.0165 (8)
O3	0.1105 (15)	0.0799 (12)	0.0767 (12)	−0.0173 (10)	0.0123 (11)	0.0047 (9)

Geometric parameters (Å, º)

C1—C3^{i}	1.373 (3)	C14—H14B	0.9700
C1—C2	1.376 (3)	C14—H14C	0.9700
C1—H1	0.9300	C14—H14D	0.9700
C2—C3	1.376 (3)	C15—C16	1.494 (8)
C2—N1	1.444 (2)	C15—H15A	0.9700
C3—C1^{i}	1.373 (3)	C15—H15B	0.9700
C3—H3	0.9300	C16—H16A	0.9600
C4—N2	1.314 (3)	C16—H16B	0.9600
C4—N3	1.340 (3)	C16—H16C	0.9600
C4—N1	1.396 (3)	C15′—C16′	1.484 (9)
C5—N2	1.356 (3)	C15′—H15C	0.9700
C5—C6	1.359 (3)	C15′—H15D	0.9700
C5—C8	1.451 (3)	C16′—H16D	0.9600
C6—O2	1.380 (2)	C16′—H16E	0.9600
C6—C7	1.406 (3)	C16′—H16F	0.9600
C7—O1	1.221 (3)	C17—C18	1.439 (7)
C7—N1	1.412 (3)	C17—H17A	0.9600
C8—C9	1.387 (4)	C17—H17B	0.9600
C8—C13	1.391 (3)	C17—H17C	0.9600
C9—O2	1.378 (3)	C18—O3	1.415 (6)
C9—C10	1.379 (3)	C18—H18A	0.9700
C10—C11	1.372 (4)	C18—H18B	0.9700
C10—H10	0.9300	C17′—C18′	1.482 (9)
C11—C12	1.386 (4)	C17′—H17D	0.9600
C11—H11	0.9300	C17′—H17E	0.9600
C12—C13	1.375 (4)	C17′—H17F	0.9600
C12—H12	0.9300	C18′—O3	1.457 (8)
C13—H13	0.9300	C18′—H18C	0.9700
C14—C15	1.442 (6)	C18′—H18D	0.9700
C14—N3	1.446 (3)	N3—H3A	0.8600
C14—C15′	1.561 (9)	O3—H3B	0.8200
C14—H14A	0.9700		
C3^{i}—C1—C2	119.50 (18)	N3—C14—H14D	111.9
C3^{i}—C1—H1	120.3	C15′—C14—H14D	112.0
C2—C1—H1	120.3	H14A—C14—H14D	17.5
C3—C2—C1	120.85 (18)	H14B—C14—H14D	89.3
C3—C2—N1	119.49 (17)	H14C—C14—H14D	109.6

C1—C2—N1	119.65 (17)	C14—C15—C16	108.0 (6)
C1^{i}—C3—C2	119.65 (18)	C14—C15—H15A	110.1
C1^{i}—C3—H3	120.2	C16—C15—H15A	110.1
C2—C3—H3	120.2	C14—C15—H15B	110.1
N2—C4—N3	120.22 (19)	C16—C15—H15B	110.1
N2—C4—N1	122.93 (19)	H15A—C15—H15B	108.4
N3—C4—N1	116.85 (18)	C16′—C15′—C14	113.9 (9)
N2—C5—C6	125.20 (19)	C16′—C15′—H15C	108.8
N2—C5—C8	129.4 (2)	C14—C15′—H15C	108.8
C6—C5—C8	105.39 (19)	C16′—C15′—H15D	108.8
C5—C6—O2	113.20 (18)	C14—C15′—H15D	108.8
C5—C6—C7	122.9 (2)	H15C—C15′—H15D	107.7
O2—C6—C7	123.9 (2)	C15′—C16′—H16D	109.5
O1—C7—C6	128.7 (2)	C15′—C16′—H16E	109.5
O1—C7—N1	121.00 (19)	H16D—C16′—H16E	109.5
C6—C7—N1	110.25 (19)	C15′—C16′—H16F	109.5
C9—C8—C13	119.0 (2)	H16D—C16′—H16F	109.5
C9—C8—C5	105.22 (19)	H16E—C16′—H16F	109.5
C13—C8—C5	135.7 (2)	O3—C18—C17	110.6 (5)
O2—C9—C10	124.5 (3)	O3—C18—H18A	109.5
O2—C9—C8	111.97 (18)	C17—C18—H18A	109.5
C10—C9—C8	123.5 (2)	O3—C18—H18B	109.5
C11—C10—C9	116.3 (3)	C17—C18—H18B	109.5
C11—C10—H10	121.8	H18A—C18—H18B	108.1
C9—C10—H10	121.8	C18′—C17′—H17D	109.5
C10—C11—C12	121.5 (2)	C18′—C17′—H17E	109.5
C10—C11—H11	119.3	H17D—C17′—H17E	109.5
C12—C11—H11	119.3	C18′—C17′—H17F	109.5
C13—C12—C11	121.7 (3)	H17D—C17′—H17F	109.5
C13—C12—H12	119.2	H17E—C17′—H17F	109.5
C11—C12—H12	119.2	O3—C18′—C17′	109.3 (9)
C12—C13—C8	117.9 (3)	O3—C18′—H18C	109.8
C12—C13—H13	121.0	C17′—C18′—H18C	109.8
C8—C13—H13	121.0	O3—C18′—H18D	109.8
C15—C14—N3	121.6 (4)	C17′—C18′—H18D	109.8
C15—C14—C15′	30.8 (5)	H18C—C18′—H18D	108.3
N3—C14—C15′	99.0 (5)	C4—N1—C7	124.16 (18)
C15—C14—H14A	106.9	C4—N1—C2	120.16 (16)
N3—C14—H14A	106.9	C7—N1—C2	115.68 (16)
C15′—C14—H14A	97.2	C4—N2—C5	114.54 (18)
C15—C14—H14B	106.9	C4—N3—C14	122.8 (2)
N3—C14—H14B	106.9	C4—N3—H3A	118.6
C15′—C14—H14B	137.2	C14—N3—H3A	118.6
H14A—C14—H14B	106.7	C9—O2—C6	104.22 (18)
C15—C14—H14C	83.4	C18—O3—C18′	31.7 (4)
N3—C14—H14C	111.9	C18—O3—H3A	124.5
C15′—C14—H14C	112.2	C18′—O3—H3A	102.6
H14A—C14—H14C	125.7	C18—O3—H3B	109.5
H14B—C14—H14C	26.1	C18′—O3—H3B	110.8

C15—C14—H14D	114.7	H3A—O3—H3B	119.4
C3^{i}—C1—C2—C3	0.2 (3)	N3—C14—C15′—C16′	179.6 (12)
C3^{i}—C1—C2—N1	178.92 (18)	N2—C4—N1—C7	2.6 (3)
C1—C2—C3—C1^{i}	−0.2 (4)	N3—C4—N1—C7	−176.89 (18)
N1—C2—C3—C1^{i}	−178.92 (18)	N2—C4—N1—C2	−177.97 (18)
N2—C5—C6—O2	−178.42 (17)	N3—C4—N1—C2	2.6 (3)
C8—C5—C6—O2	0.5 (2)	O1—C7—N1—C4	179.69 (19)
N2—C5—C6—C7	0.2 (3)	C6—C7—N1—C4	−0.5 (3)
C8—C5—C6—C7	179.07 (19)	O1—C7—N1—C2	0.2 (3)
C5—C6—C7—O1	179.0 (2)	C6—C7—N1—C2	180.00 (17)
O2—C6—C7—O1	−2.5 (4)	C3—C2—N1—C4	−101.3 (2)
C5—C6—C7—N1	−0.7 (3)	C1—C2—N1—C4	80.0 (2)
O2—C6—C7—N1	177.70 (18)	C3—C2—N1—C7	78.2 (2)
N2—C5—C8—C9	178.42 (19)	C1—C2—N1—C7	−100.5 (2)
C6—C5—C8—C9	−0.4 (2)	N3—C4—N2—C5	176.47 (18)
N2—C5—C8—C13	−0.4 (4)	N1—C4—N2—C5	−3.0 (3)
C6—C5—C8—C13	−179.3 (2)	C6—C5—N2—C4	1.7 (3)
C13—C8—C9—O2	179.31 (18)	C8—C5—N2—C4	−176.91 (18)
C5—C8—C9—O2	0.2 (2)	N2—C4—N3—C14	0.8 (3)
C13—C8—C9—C10	−1.3 (3)	N1—C4—N3—C14	−179.7 (2)
C5—C8—C9—C10	179.6 (2)	C15—C14—N3—C4	81.6 (4)
O2—C9—C10—C11	179.4 (2)	C15′—C14—N3—C4	104.2 (8)
C8—C9—C10—C11	0.1 (3)	C10—C9—O2—C6	−179.3 (2)
C9—C10—C11—C12	0.7 (4)	C8—C9—O2—C6	0.0 (2)
C10—C11—C12—C13	−0.2 (4)	C5—C6—O2—C9	−0.3 (2)
C11—C12—C13—C8	−0.9 (3)	C7—C6—O2—C9	−178.9 (2)
C9—C8—C13—C12	1.6 (3)	C17—C18—O3—C18′	44.0 (11)
C5—C8—C13—C12	−179.6 (2)	C17—C18—O3—H3A	−8.6
N3—C14—C15—C16	68.1 (6)	C17′—C18′—O3—C18	−29.5 (10)
C15′—C14—C15—C16	20.3 (14)	C17′—C18′—O3—H3A	108.4
C15—C14—C15′—C16′	−40.1 (9)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3a···O3	0.86	2.22	2.996 (3)	150
O3—H3b···O1^{i}	0.82	2.12	2.903 (3)	159

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