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1-[2-(4-Chlorobenzyloxy)-2-phenylethyl]-1*H*-benzotriazole

Özden Özel Güven,[a] Meral Bayraktar,[a] Simon J. Coles[b] and Tuncer Hökelek[c]*

[a]Department of Chemistry, Zonguldak Karaelmas University, 67100 Zonguldak, Turkey, [b]Department of Chemistry, Southampton University, Southampton SO17 1BJ, England, and [c]Department of Physics, Hacettepe University, 06800 Beytepe, Ankara, Turkey
Correspondence e-mail: merzifon@hacettepe.edu.tr

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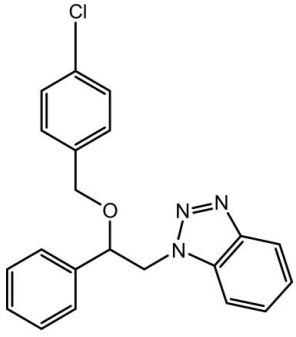
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.003 Å; R factor = 0.065; wR factor = 0.189; data-to-parameter ratio = 17.0.

The asymmetric unit of the title compound, $C_{21}H_{18}ClN_3O$, contains two crystallographically independent molecules which differ slightly in the orientations of chlorobenzyloxy units. In one of the molecules, the phenyl and chlorophenyl rings are oriented at dihedral angles of 38.09 (6) and 42.15 (6)°, respectively, with respect to the benzotriazole ring [43.23 (6) and 29.80 (6)° in the other molecule]. The dihedral angle between the phenyl and chlorophenyl rings is 77.63 (6)° in one of the molecules and 72.97 (6)° in the other. The crystal structure is stabilized by weak C—H$\cdots\pi$ interactions.

Related literature

For general background to the biological activity of benzotriazole derivatives, see: Hirokawa *et al.* (1998); Yu *et al.* (2003); Kopanska *et al.* (2004). For related structures, see: Caira *et al.* (2004); Freer *et al.* (1986); Katritzky *et al.* (2001); Özel Güven *et al.* (2007*a*,*b*, 2008*a*,*b*,*c*, 2010); Peeters *et al.* (1979*a*,*b*, 1996); Swamy *et al.* (2006).



Experimental

Crystal data

$C_{21}H_{18}ClN_3O$
M_r = 363.83
Monoclinic, $P2_1/c$
a = 7.2163 (2) Å
b = 36.8545 (9) Å
c = 13.3019 (3) Å
β = 91.529 (1)°
V = 3536.42 (15) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 120 K
0.40 × 0.40 × 0.14 mm

Data collection

Nonius Kappa CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
T_{min} = 0.910, T_{max} = 0.966
26731 measured reflections
7993 independent reflections
5918 reflections with $I > 2\sigma(I)$
R_{int} = 0.051

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.189
S = 1.07
7993 reflections
470 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.64 e Å^{-3}
$\Delta\rho_{min}$ = −0.69 e Å^{-3}

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

*Cg*1, *Cg*2 and *Cg*3 are centroids of the C9–C14, C9′–C14′ and C16–C21 rings, respectively.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C11—H11$\cdots Cg2^{i}$	0.95	2.62	3.515 (2)	157
C11′—H11′$\cdots Cg1^{ii}$	0.95	2.79	3.635 (2)	149
C14—H14$\cdots Cg2^{iii}$	0.95	2.64	3.584 (2)	172
C14′—H14′$\cdots Cg1^{iv}$	0.95	2.81	3.755 (2)	172
C18′—H18′$\cdots Cg3^{v}$	0.95	2.83	3.502 (2)	129

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

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; 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, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI5085).

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1-[2-(4-Chlorobenzyloxy)-2-phenylethyl]-1*H*-benzotriazole

Özden Özel Güven, Meral Bayraktar, Simon J. Coles and Tuncer Hökelek

S1. Comment

In recent years, there has been increasing interest in the syntheses of heterocyclic compounds that have biological and commercial importance. Clotrimazole, miconazole, econazole, ketonazole, itraconazole and fluconazole are well-known imidazoles. 1*H*-1,2,4-Triazole ring containing azole derivatives have been developed for clinical uses as antifungal agents. Recently, structures containing benzimidazole ring in place of miconazole and econazole have been reported, and these molecules have been shown more antibacterial activity than antifungal activity (Özel Güven *et al.*, 2007a,b). The crystal structures of miconazole (Peeters *et al.*, 1979a), ketonazole (Peeters *et al.*, 1979b), econazole (Freer *et al.*, 1986), itraconazole (Peeters *et al.*, 1996) and fluconazole (Caira *et al.*, 2004) have been reported. Recently, we reported crystal structures of related compounds (Özel Güven *et al.*, 2008a,b,c). Benzotriazole derivatives also exhibit a good degree of analgesic, antiinflammatory, diuretic, antiviral and antihypertensive activities (Hirokawa *et al.*, 1998; Yu *et al.*, 2003; Kopanska *et al.*, 2004). Crystal structures of benzotriazole ring possessing compounds have been reported (Katritzky *et al.*, 2001; Swamy *et al.*, 2006; Özel Güven *et al.*, 2010). Now, we report herein the crystal structure of the title benzotriazole derivative.

The asymmetric unit of the title compound (Fig. 1) contains two crystallographically independent molecules which differ slightly in the orientations of the chlorobenzyloxy units. The bond lengths and angles are generally within normal ranges. In each molecule, the planar benzotriazole rings [A (N1-N3/C1-C6) and A′ (N1′-N3′/C1′-C6′)] are oriented with respect to the phenyl [B (C9-C14) and B′ (C9′-C14′)] and benzene [C (C16-C21)] and C′ (C16′-C21′)] rings at dihedral angles of A/B = 37.98 (9), A/C = 42.27 (9) ° and A′/B′ = 43.20 (9), A′/C′ = 29.82 (9)°. The dihedral angles between phenyl and benzene rings are B/C = 77.63 (6) and B′/C′ = 72.97 (6) °. Atoms C7 and C7′ are -0.012 (2) and -0.112 (2) Å away from the planes of the benzotriazole rings, respectively.

In the crystal structure, molecules are stacked along the a-axis (Fig. 2). Weak C—H···π interactions (Table 1) involving the C9-C14, C9′-C14′ and C16-C21 rings stabilize the structure.

S2. Experimental

The title compound was synthesized by the reaction of 2-(1*H*-benzotriazol-1-yl)-1-phenylethanol (Özel Güven *et al.*, 2010) with aryl halide using NaH. 2-(1*H*-Benzotriazol-1-yl)-1-phenylethanol (200 mg, 0.84 mmol) was dissolved in DMF (4 ml). NaH (33 mg, 0.84 mmol) was added to the solution portionwise. After stirring the mixture a few minutes, 4-chlorobenzyl bromide (171.8 mg, 0.84 mmol) was added dropwise. Then, the reaction mixture was stirred additional 3 h at room temperature. The reaction was stopped by adding methanol (5 ml). After evaporation of the solvent, dichloromethane was added to the reaction mixture and extracted with water. Then, the organic phase was separated, dried, filtered and evaporated. The precipitate formed was purified by column chromatography using chloroform and crystallized from *iso*-propanol to obtain colorless crystals suitable for X-ray analysis (yield; 137 mg, 46%).

S3. Refinement

H atoms were positioned geometrically with C-H = 0.95, 1.00 and 0.99 Å for aromatic, methine and methylene H, respectively, and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.

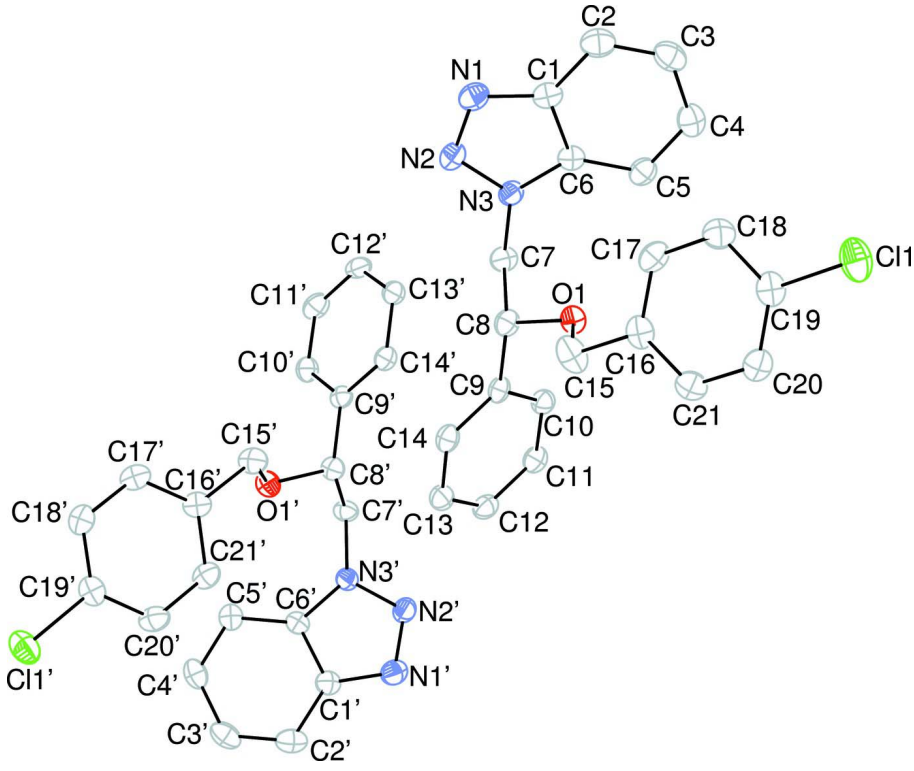

Figure 1

The two independent molecules of the title compound, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity.

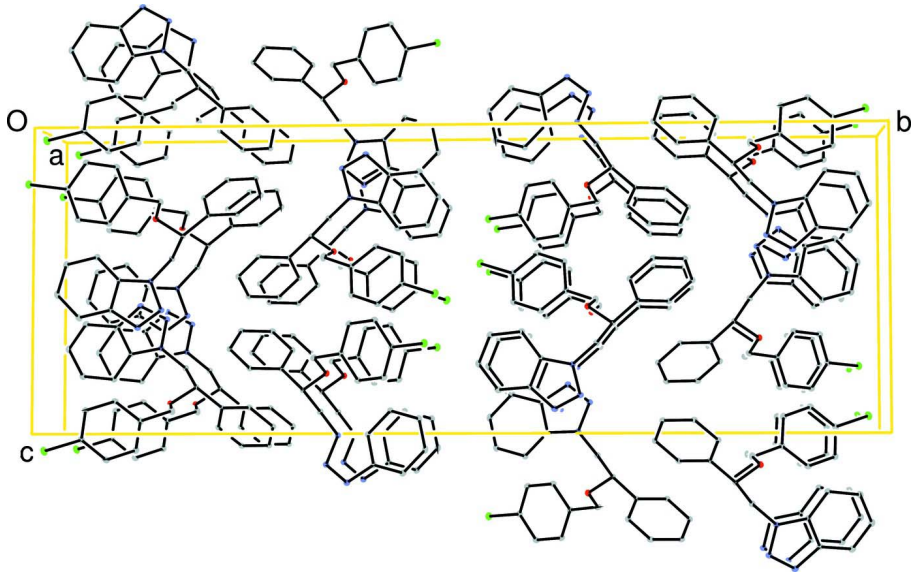

Figure 2

Packing diagram of the title compound, viewed along the *a* axis. H atoms have been omitted for clarity.

1-[2-(4-Chlorobenzyloxy)-2-phenylethyl]-1*H*-benzotriazole

Crystal data

$C_{21}H_{18}ClN_3O$
$M_r = 363.83$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 7.2163\ (2)$ Å
$b = 36.8545\ (9)$ Å
$c = 13.3019\ (3)$ Å
$\beta = 91.529\ (1)°$
$V = 3536.42\ (15)$ Å^3
$Z = 8$
$F(000) = 1520$
$D_x = 1.367$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 26277 reflections
$\theta = 2.9–27.5°$
$\mu = 0.23$ mm^{-1}
$T = 120$ K
Slab, colourless
0.40 × 0.40 × 0.14 mm

Data collection

Nonius Kappa CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
$T_{min} = 0.910$, $T_{max} = 0.966$
26731 measured reflections
7993 independent reflections
5918 reflections with $I > 2\sigma(I)$
$R_{int} = 0.051$
$\theta_{max} = 27.6°$, $\theta_{min} = 3.0°$
$h = -9\rightarrow9$
$k = -47\rightarrow43$
$l = -17\rightarrow17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.065$
$wR(F^2) = 0.189$
$S = 1.07$
7993 reflections
470 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
$w = 1/[\sigma^2(F_o^2) + (0.1171P)^2 + 0.2599P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.64$ e Å^{-3}
$\Delta\rho_{min} = -0.69$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.038 (2)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2$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	−0.22475 (9)	0.476481 (18)	0.55416 (6)	0.0416 (2)
O1	0.3382 (2)	0.34725 (4)	0.40142 (11)	0.0230 (3)
N1	0.3727 (3)	0.38511 (5)	0.07784 (14)	0.0288 (5)
N2	0.4375 (3)	0.35556 (5)	0.12052 (14)	0.0269 (4)
N3	0.4929 (3)	0.36393 (5)	0.21634 (13)	0.0228 (4)
C1	0.3846 (3)	0.41288 (6)	0.14623 (17)	0.0250 (5)
C2	0.3361 (3)	0.44961 (7)	0.13830 (19)	0.0327 (6)
H2	0.2799	0.4591	0.0785	0.039*
C3	0.3729 (3)	0.47135 (7)	0.2200 (2)	0.0330 (6)
H3	0.3418	0.4964	0.2166	0.040*
C4	0.4559 (3)	0.45739 (7)	0.30917 (19)	0.0313 (5)
H4	0.4821	0.4734	0.3636	0.038*
C5	0.4999 (3)	0.42131 (6)	0.31946 (17)	0.0264 (5)
H5	0.5527	0.4118	0.3801	0.032*
C6	0.4626 (3)	0.39944 (6)	0.23575 (16)	0.0222 (5)
C7	0.5705 (3)	0.33638 (6)	0.28229 (17)	0.0250 (5)
H7A	0.6674	0.3474	0.3266	0.030*
H7B	0.6299	0.3174	0.2414	0.030*
C8	0.4235 (3)	0.31891 (6)	0.34680 (16)	0.0239 (5)
H8	0.3278	0.3074	0.3014	0.029*
C9	0.5062 (3)	0.29013 (6)	0.41518 (15)	0.0209 (5)
C10	0.6548 (3)	0.29873 (6)	0.48017 (16)	0.0234 (5)
H10	0.7022	0.3228	0.4821	0.028*
C11	0.7333 (3)	0.27231 (6)	0.54186 (16)	0.0259 (5)
H11	0.8358	0.2782	0.5851	0.031*
C12	0.6629 (3)	0.23736 (6)	0.54066 (16)	0.0254 (5)
H12	0.7166	0.2193	0.5833	0.030*
C13	0.5145 (3)	0.22873 (6)	0.47732 (16)	0.0248 (5)
H13	0.4654	0.2048	0.4769	0.030*
C14	0.4368 (3)	0.25505 (6)	0.41408 (16)	0.0233 (5)
H14	0.3359	0.2489	0.3700	0.028*
C15	0.1497 (3)	0.33957 (7)	0.4250 (2)	0.0360 (6)
H15A	0.1459	0.3212	0.4791	0.043*
H15B	0.0831	0.3297	0.3649	0.043*
C16	0.0583 (3)	0.37382 (6)	0.45829 (18)	0.0265 (5)
C17	0.0463 (3)	0.40358 (7)	0.39399 (17)	0.0273 (5)
H17	0.0966	0.4020	0.3288	0.033*
C18	−0.0374 (3)	0.43532 (6)	0.42360 (18)	0.0291 (5)
H18	−0.0430	0.4557	0.3799	0.035*
C19	−0.1137 (3)	0.43699 (6)	0.51846 (18)	0.0278 (5)
C20	−0.1040 (3)	0.40812 (6)	0.58310 (18)	0.0276 (5)
H20	−0.1553	0.4097	0.6480	0.033*
C21	−0.0178 (3)	0.37633 (6)	0.55244 (18)	0.0272 (5)
H21	−0.0113	0.3561	0.5967	0.033*
Cl1′	0.19246 (9)	0.026883 (16)	0.22027 (5)	0.0384 (2)

O1′	0.8366 (2)	0.15017 (4)	0.30657 (11)	0.0248 (4)
N1′	0.9026 (3)	0.12718 (5)	0.65649 (14)	0.0294 (5)
N2′	0.9650 (3)	0.15280 (5)	0.59942 (14)	0.0274 (4)
N3′	0.9881 (3)	0.13952 (5)	0.50553 (13)	0.0225 (4)
C1′	0.8871 (3)	0.09601 (6)	0.59982 (17)	0.0247 (5)
C2′	0.8299 (3)	0.06087 (7)	0.62520 (19)	0.0307 (5)
H2′	0.7928	0.0551	0.6913	0.037*
C3′	0.8297 (3)	0.03530 (6)	0.5510 (2)	0.0320 (6)
H3′	0.7897	0.0114	0.5658	0.038*
C4′	0.8873 (3)	0.04340 (6)	0.45265 (19)	0.0296 (5)
H4′	0.8868	0.0247	0.4035	0.036*
C5′	0.9438 (3)	0.07756 (6)	0.42656 (17)	0.0253 (5)
H5′	0.9818	0.0831	0.3605	0.030*
C6′	0.9424 (3)	0.10373 (6)	0.50228 (16)	0.0211 (4)
C7′	1.0704 (3)	0.16200 (6)	0.42962 (16)	0.0235 (5)
H7C	1.1558	0.1471	0.3898	0.028*
H7D	1.1442	0.1814	0.4629	0.028*
C8′	0.9260 (3)	0.17904 (6)	0.35944 (16)	0.0226 (5)
H8′	0.8322	0.1917	0.4010	0.027*
C9′	1.0112 (3)	0.20660 (6)	0.29009 (15)	0.0207 (4)
C10′	1.1563 (3)	0.19730 (6)	0.22767 (17)	0.0241 (5)
H10′	1.2023	0.1731	0.2278	0.029*
C11′	1.2337 (3)	0.22296 (7)	0.16565 (17)	0.0290 (5)
H11′	1.3332	0.2165	0.1239	0.035*
C12′	1.1663 (3)	0.25810 (6)	0.16425 (16)	0.0262 (5)
H12′	1.2187	0.2757	0.1212	0.031*
C13′	1.0226 (3)	0.26762 (6)	0.22557 (16)	0.0243 (5)
H13′	0.9763	0.2917	0.2244	0.029*
C14′	0.9455 (3)	0.24203 (6)	0.28896 (16)	0.0228 (5)
H14′	0.8477	0.2488	0.3316	0.027*
C15′	0.6640 (3)	0.16060 (6)	0.25888 (18)	0.0287 (5)
H15C	0.6864	0.1714	0.1922	0.034*
H15D	0.6006	0.1788	0.3005	0.034*
C16′	0.5460 (3)	0.12733 (6)	0.24718 (17)	0.0246 (5)
C17′	0.4741 (3)	0.11645 (7)	0.15453 (17)	0.0265 (5)
H17′	0.4985	0.1305	0.0965	0.032*
C18′	0.3671 (3)	0.08540 (6)	0.14502 (18)	0.0267 (5)
H18′	0.3189	0.0780	0.0811	0.032*
C19′	0.3319 (3)	0.06545 (6)	0.23027 (18)	0.0272 (5)
C20′	0.4002 (3)	0.07576 (7)	0.32357 (18)	0.0303 (5)
H20′	0.3738	0.0617	0.3814	0.036*
C21′	0.5076 (3)	0.10674 (7)	0.33240 (17)	0.0268 (5)
H21′	0.5553	0.1140	0.3965	0.032*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0341 (4)	0.0352 (4)	0.0555 (5)	0.0105 (3)	0.0044 (3)	−0.0115 (3)

O1	0.0185 (8)	0.0235 (8)	0.0271 (8)	−0.0002 (6)	0.0016 (6)	−0.0028 (6)
N1	0.0275 (11)	0.0344 (11)	0.0244 (10)	0.0009 (9)	−0.0033 (8)	0.0026 (9)
N2	0.0290 (11)	0.0310 (11)	0.0205 (10)	−0.0007 (8)	−0.0004 (8)	−0.0020 (8)
N3	0.0245 (10)	0.0243 (9)	0.0197 (9)	0.0029 (7)	0.0006 (7)	0.0003 (7)
C1	0.0201 (11)	0.0300 (12)	0.0249 (11)	−0.0002 (9)	0.0007 (9)	0.0042 (9)
C2	0.0273 (13)	0.0369 (14)	0.0339 (13)	0.0034 (10)	−0.0004 (10)	0.0076 (11)
C3	0.0301 (13)	0.0263 (12)	0.0428 (15)	0.0051 (10)	0.0040 (11)	0.0040 (11)
C4	0.0260 (12)	0.0310 (13)	0.0371 (14)	−0.0006 (10)	0.0045 (10)	−0.0057 (11)
C5	0.0234 (12)	0.0318 (12)	0.0241 (11)	−0.0007 (9)	0.0035 (9)	−0.0004 (9)
C6	0.0182 (10)	0.0247 (11)	0.0239 (11)	0.0010 (9)	0.0018 (9)	0.0026 (9)
C7	0.0236 (11)	0.0264 (11)	0.0252 (11)	0.0053 (9)	0.0034 (9)	0.0025 (9)
C8	0.0219 (11)	0.0268 (11)	0.0229 (11)	0.0025 (9)	0.0012 (9)	−0.0021 (9)
C9	0.0185 (11)	0.0250 (11)	0.0193 (10)	0.0029 (8)	0.0031 (8)	−0.0047 (9)
C10	0.0246 (11)	0.0241 (11)	0.0215 (11)	0.0014 (9)	0.0025 (9)	−0.0010 (9)
C11	0.0256 (12)	0.0306 (12)	0.0215 (11)	0.0004 (9)	−0.0023 (9)	−0.0023 (9)
C12	0.0280 (12)	0.0278 (12)	0.0205 (11)	0.0059 (9)	0.0038 (9)	0.0013 (9)
C13	0.0251 (12)	0.0247 (11)	0.0248 (11)	−0.0002 (9)	0.0058 (9)	−0.0023 (9)
C14	0.0198 (11)	0.0282 (11)	0.0219 (11)	0.0007 (9)	0.0012 (8)	−0.0048 (9)
C15	0.0226 (12)	0.0290 (13)	0.0569 (17)	−0.0013 (10)	0.0100 (11)	−0.0076 (12)
C16	0.0157 (11)	0.0286 (12)	0.0350 (13)	−0.0019 (9)	−0.0002 (9)	−0.0056 (10)
C17	0.0203 (11)	0.0381 (13)	0.0237 (11)	0.0015 (10)	0.0027 (9)	−0.0016 (10)
C18	0.0254 (12)	0.0308 (12)	0.0310 (13)	0.0051 (10)	−0.0034 (10)	0.0038 (10)
C19	0.0186 (11)	0.0300 (12)	0.0348 (13)	0.0012 (9)	−0.0003 (9)	−0.0056 (10)
C20	0.0201 (11)	0.0342 (13)	0.0285 (12)	−0.0028 (9)	0.0032 (9)	−0.0037 (10)
C21	0.0193 (11)	0.0288 (12)	0.0336 (13)	−0.0038 (9)	0.0023 (9)	0.0026 (10)
Cl1′	0.0379 (4)	0.0285 (3)	0.0483 (4)	−0.0063 (3)	−0.0066 (3)	0.0003 (3)
O1′	0.0202 (8)	0.0246 (8)	0.0295 (9)	−0.0014 (6)	−0.0015 (6)	−0.0010 (7)
N1′	0.0327 (11)	0.0292 (10)	0.0267 (10)	0.0066 (9)	0.0044 (8)	0.0024 (8)
N2′	0.0342 (11)	0.0265 (10)	0.0216 (10)	0.0032 (8)	0.0005 (8)	−0.0014 (8)
N3′	0.0248 (10)	0.0205 (9)	0.0220 (9)	−0.0007 (7)	−0.0009 (7)	0.0005 (7)
C1′	0.0231 (11)	0.0235 (11)	0.0275 (12)	0.0040 (9)	0.0028 (9)	0.0016 (9)
C2′	0.0249 (12)	0.0323 (13)	0.0351 (13)	0.0054 (10)	0.0068 (10)	0.0099 (11)
C3′	0.0243 (12)	0.0230 (11)	0.0489 (15)	0.0012 (9)	0.0029 (11)	0.0054 (11)
C4′	0.0264 (12)	0.0226 (11)	0.0398 (14)	0.0019 (9)	−0.0020 (10)	−0.0054 (10)
C5′	0.0222 (11)	0.0261 (12)	0.0276 (12)	0.0023 (9)	−0.0015 (9)	−0.0019 (9)
C6′	0.0180 (10)	0.0200 (10)	0.0253 (11)	0.0013 (8)	−0.0003 (8)	0.0018 (9)
C7′	0.0221 (11)	0.0245 (11)	0.0240 (11)	−0.0042 (9)	−0.0012 (9)	0.0044 (9)
C8′	0.0201 (11)	0.0236 (11)	0.0239 (11)	−0.0009 (9)	−0.0014 (9)	0.0005 (9)
C9′	0.0188 (10)	0.0241 (11)	0.0191 (10)	−0.0010 (8)	−0.0031 (8)	0.0007 (9)
C10′	0.0225 (11)	0.0244 (11)	0.0254 (11)	0.0015 (9)	−0.0003 (9)	−0.0029 (9)
C11′	0.0234 (12)	0.0401 (14)	0.0238 (12)	−0.0014 (10)	0.0050 (9)	−0.0011 (10)
C12′	0.0270 (12)	0.0324 (12)	0.0191 (11)	−0.0086 (10)	−0.0023 (9)	0.0053 (9)
C13′	0.0274 (12)	0.0237 (11)	0.0217 (11)	−0.0026 (9)	−0.0049 (9)	0.0002 (9)
C14′	0.0227 (11)	0.0255 (11)	0.0202 (11)	−0.0002 (9)	−0.0014 (8)	−0.0017 (9)
C15′	0.0226 (12)	0.0334 (13)	0.0298 (12)	−0.0030 (10)	−0.0054 (9)	0.0052 (10)
C16′	0.0166 (10)	0.0295 (12)	0.0277 (12)	0.0022 (9)	0.0008 (9)	0.0035 (10)
C17′	0.0186 (11)	0.0360 (13)	0.0250 (12)	0.0022 (9)	−0.0001 (9)	0.0057 (10)
C18′	0.0211 (11)	0.0325 (12)	0.0264 (11)	0.0035 (9)	−0.0022 (9)	−0.0038 (10)

C19′	0.0210 (11)	0.0260 (11)	0.0346 (13)	0.0010 (9)	−0.0015 (10)	−0.0023 (10)
C20′	0.0265 (12)	0.0382 (14)	0.0264 (12)	−0.0035 (10)	0.0015 (9)	0.0063 (10)
C21′	0.0214 (11)	0.0355 (13)	0.0233 (11)	−0.0013 (9)	−0.0012 (9)	0.0010 (10)

Geometric parameters (Å, º)

Cl1—C19	1.734 (2)	Cl1′—C19′	1.745 (2)
O1—C8	1.422 (3)	O1′—C8′	1.421 (3)
O1—C15	1.432 (3)	O1′—C15′	1.435 (3)
N1—N2	1.309 (3)	N1′—N2′	1.299 (3)
N1—C1	1.371 (3)	N1′—C1′	1.377 (3)
N2—N3	1.361 (2)	N2′—N3′	1.356 (3)
N3—C6	1.353 (3)	N3′—C6′	1.360 (3)
N3—C7	1.445 (3)	N3′—C7′	1.446 (3)
C1—C6	1.394 (3)	C1′—C6′	1.397 (3)
C1—C2	1.401 (3)	C1′—C2′	1.403 (3)
C2—C3	1.371 (4)	C2′—C3′	1.365 (4)
C2—H2	0.95	C2′—H2′	0.95
C3—C4	1.411 (3)	C3′—C4′	1.415 (3)
C3—H3	0.95	C3′—H3′	0.95
C4—C5	1.373 (3)	C4′—C5′	1.371 (3)
C4—H4	0.95	C4′—H4′	0.95
C5—C6	1.395 (3)	C5′—C6′	1.395 (3)
C5—H5	0.95	C5′—H5′	0.9500
C7—C8	1.525 (3)	C7′—C8′	1.516 (3)
C7—H7A	0.99	C7′—H7C	0.99
C7—H7B	0.99	C7′—H7D	0.99
C8—C9	1.510 (3)	C8′—C9′	1.514 (3)
C8—H8	1.00	C8′—H8′	1.00
C9—C14	1.387 (3)	C9′—C14′	1.389 (3)
C9—C10	1.396 (3)	C9′—C10′	1.397 (3)
C10—C11	1.385 (3)	C10′—C11′	1.382 (3)
C10—H10	0.95	C10′—H10′	0.95
C11—C12	1.385 (3)	C11′—C12′	1.383 (3)
C11—H11	0.95	C11′—H11′	0.95
C12—C13	1.382 (3)	C12′—C13′	1.381 (3)
C12—H12	0.95	C12′—H12′	0.95
C13—C14	1.392 (3)	C13′—C14′	1.391 (3)
C13—H13	0.95	C13′—H13′	0.95
C14—H14	0.95	C14′—H14′	0.95
C15—C16	1.497 (3)	C15′—C16′	1.498 (3)
C15—H15A	0.99	C15′—H15C	0.99
C15—H15B	0.99	C15′—H15D	0.99
C16—C21	1.384 (3)	C16′—C17′	1.384 (3)
C16—C17	1.392 (3)	C16′—C21′	1.398 (3)
C17—C18	1.379 (3)	C17′—C18′	1.384 (3)
C17—H17	0.95	C17′—H17′	0.95
C18—C19	1.391 (3)	C18′—C19′	1.380 (3)

C18—H18	0.95	C18′—H18′	0.95
C19—C20	1.369 (3)	C19′—C20′	1.377 (3)
C20—C21	1.393 (3)	C20′—C21′	1.383 (3)
C20—H20	0.95	C20′—H20′	0.95
C21—H21	0.95	C21′—H21′	0.95
C8—O1—C15	113.13 (17)	C8′—O1′—C15′	113.31 (17)
N2—N1—C1	108.55 (18)	N2′—N1′—C1′	108.11 (18)
N1—N2—N3	108.07 (18)	N1′—N2′—N3′	109.20 (18)
C6—N3—N2	110.69 (17)	N2′—N3′—C6′	110.10 (18)
C6—N3—C7	128.75 (18)	N2′—N3′—C7′	119.96 (18)
N2—N3—C7	120.56 (18)	C6′—N3′—C7′	129.59 (19)
N1—C1—C6	108.6 (2)	N1′—C1′—C6′	108.51 (19)
N1—C1—C2	131.3 (2)	N1′—C1′—C2′	131.2 (2)
C6—C1—C2	120.1 (2)	C6′—C1′—C2′	120.3 (2)
C3—C2—C1	117.5 (2)	C3′—C2′—C1′	117.2 (2)
C3—C2—H2	121.2	C3′—C2′—H2′	121.4
C1—C2—H2	121.2	C1′—C2′—H2′	121.4
C2—C3—C4	121.5 (2)	C2′—C3′—C4′	121.9 (2)
C2—C3—H3	119.3	C2′—C3′—H3′	119.0
C4—C3—H3	119.3	C4′—C3′—H3′	119.0
C5—C4—C3	121.9 (2)	C5′—C4′—C3′	121.6 (2)
C5—C4—H4	119.0	C5′—C4′—H4′	119.2
C3—C4—H4	119.0	C3′—C4′—H4′	119.2
C4—C5—C6	116.2 (2)	C4′—C5′—C6′	116.4 (2)
C4—C5—H5	121.9	C4′—C5′—H5′	121.8
C6—C5—H5	121.9	C6′—C5′—H5′	121.8
N3—C6—C1	104.13 (19)	N3′—C6′—C5′	133.4 (2)
N3—C6—C5	133.0 (2)	N3′—C6′—C1′	104.07 (19)
C1—C6—C5	122.8 (2)	C5′—C6′—C1′	122.5 (2)
N3—C7—C8	111.97 (18)	N3′—C7′—C8′	112.26 (18)
N3—C7—H7A	109.2	N3′—C7′—H7C	109.2
C8—C7—H7A	109.2	C8′—C7′—H7C	109.2
N3—C7—H7B	109.2	N3′—C7′—H7D	109.2
C8—C7—H7B	109.2	C8′—C7′—H7D	109.2
H7A—C7—H7B	107.9	H7C—C7′—H7D	107.9
O1—C8—C9	112.19 (17)	O1′—C8′—C9′	112.79 (17)
O1—C8—C7	107.12 (17)	O1′—C8′—C7′	106.87 (17)
C9—C8—C7	111.46 (18)	C9′—C8′—C7′	111.70 (18)
O1—C8—H8	108.7	O1′—C8′—H8′	108.4
C9—C8—H8	108.7	C9′—C8′—H8′	108.4
C7—C8—H8	108.7	C7′—C8′—H8′	108.4
C14—C9—C10	119.3 (2)	C14′—C9′—C10′	119.0 (2)
C14—C9—C8	120.78 (19)	C14′—C9′—C8′	119.57 (19)
C10—C9—C8	119.91 (19)	C10′—C9′—C8′	121.38 (19)
C11—C10—C9	120.2 (2)	C11′—C10′—C9′	120.5 (2)
C11—C10—H10	119.9	C11′—C10′—H10′	119.7
C9—C10—H10	119.9	C9′—C10′—H10′	119.7

C12—C11—C10	120.2 (2)	C10′—C11′—C12′	120.1 (2)
C12—C11—H11	119.9	C10′—C11′—H11′	120.0
C10—C11—H11	119.9	C12′—C11′—H11′	120.0
C13—C12—C11	120.0 (2)	C13′—C12′—C11′	119.9 (2)
C13—C12—H12	120.0	C13′—C12′—H12′	120.0
C11—C12—H12	120.0	C11′—C12′—H12′	120.0
C12—C13—C14	120.1 (2)	C12′—C13′—C14′	120.3 (2)
C12—C13—H13	120.0	C12′—C13′—H13′	119.9
C14—C13—H13	120.0	C14′—C13′—H13′	119.9
C9—C14—C13	120.3 (2)	C9′—C14′—C13′	120.1 (2)
C9—C14—H14	119.9	C9′—C14′—H14′	119.9
C13—C14—H14	119.9	C13′—C14′—H14′	119.9
O1—C15—C16	109.06 (18)	O1′—C15′—C16′	108.11 (18)
O1—C15—H15A	109.9	O1′—C15′—H15C	110.1
C16—C15—H15A	109.9	C16′—C15′—H15C	110.1
O1—C15—H15B	109.9	O1′—C15′—H15D	110.1
C16—C15—H15B	109.9	C16′—C15′—H15D	110.1
H15A—C15—H15B	108.3	H15C—C15′—H15D	108.4
C21—C16—C17	118.9 (2)	C17′—C16′—C21′	119.1 (2)
C21—C16—C15	120.9 (2)	C17′—C16′—C15′	121.9 (2)
C17—C16—C15	120.2 (2)	C21′—C16′—C15′	119.0 (2)
C18—C17—C16	120.9 (2)	C16′—C17′—C18′	121.1 (2)
C18—C17—H17	119.6	C16′—C17′—H17′	119.5
C16—C17—H17	119.6	C18′—C17′—H17′	119.5
C17—C18—C19	118.9 (2)	C19′—C18′—C17′	118.6 (2)
C17—C18—H18	120.5	C19′—C18′—H18′	120.7
C19—C18—H18	120.5	C17′—C18′—H18′	120.7
C20—C19—C18	121.4 (2)	C20′—C19′—C18′	121.6 (2)
C20—C19—Cl1	119.79 (18)	C20′—C19′—Cl1′	119.05 (18)
C18—C19—Cl1	118.85 (19)	C18′—C19′—Cl1′	119.30 (18)
C19—C20—C21	119.1 (2)	C19′—C20′—C21′	119.4 (2)
C19—C20—H20	120.5	C19′—C20′—H20′	120.3
C21—C20—H20	120.5	C21′—C20′—H20′	120.3
C16—C21—C20	120.8 (2)	C20′—C21′—C16′	120.1 (2)
C16—C21—H21	119.6	C20′—C21′—H21′	119.9
C20—C21—H21	119.6	C16′—C21′—H21′	119.9

C1—N1—N2—N3	−0.4 (2)	C1′—N1′—N2′—N3′	1.1 (2)
N1—N2—N3—C6	0.2 (2)	N1′—N2′—N3′—C6′	−1.2 (2)
N1—N2—N3—C7	179.79 (19)	N1′—N2′—N3′—C7′	−175.07 (19)
N2—N1—C1—C6	0.4 (3)	N2′—N1′—C1′—C6′	−0.6 (3)
N2—N1—C1—C2	179.3 (2)	N2′—N1′—C1′—C2′	178.9 (2)
N1—C1—C2—C3	−177.2 (2)	N1′—C1′—C2′—C3′	−179.9 (2)
C6—C1—C2—C3	1.7 (3)	C6′—C1′—C2′—C3′	−0.5 (3)
C1—C2—C3—C4	−0.2 (4)	C1′—C2′—C3′—C4′	1.0 (4)
C2—C3—C4—C5	−1.6 (4)	C2′—C3′—C4′—C5′	−1.0 (4)
C3—C4—C5—C6	1.7 (3)	C3′—C4′—C5′—C6′	0.4 (3)
N2—N3—C6—C1	0.1 (2)	N2′—N3′—C6′—C5′	−178.8 (2)

C7—N3—C6—C1	−179.5 (2)	C7′—N3′—C6′—C5′	−5.7 (4)
N2—N3—C6—C5	−177.4 (2)	N2′—N3′—C6′—C1′	0.8 (2)
C7—N3—C6—C5	3.0 (4)	C7′—N3′—C6′—C1′	173.9 (2)
N1—C1—C6—N3	−0.3 (2)	C4′—C5′—C6′—N3′	179.7 (2)
C2—C1—C6—N3	−179.4 (2)	C4′—C5′—C6′—C1′	0.1 (3)
N1—C1—C6—C5	177.6 (2)	N1′—C1′—C6′—N3′	−0.2 (2)
C2—C1—C6—C5	−1.5 (3)	C2′—C1′—C6′—N3′	−179.7 (2)
C4—C5—C6—N3	176.9 (2)	N1′—C1′—C6′—C5′	179.5 (2)
C4—C5—C6—C1	−0.2 (3)	C2′—C1′—C6′—C5′	0.0 (3)
C6—N3—C7—C8	85.9 (3)	N2′—N3′—C7′—C8′	−99.2 (2)
N2—N3—C7—C8	−93.6 (2)	C6′—N3′—C7′—C8′	88.3 (3)
C15—O1—C8—C9	−86.2 (2)	C15′—O1′—C8′—C9′	−73.5 (2)
C15—O1—C8—C7	151.18 (19)	C15′—O1′—C8′—C7′	163.40 (18)
N3—C7—C8—O1	−57.0 (2)	N3′—C7′—C8′—O1′	−64.4 (2)
N3—C7—C8—C9	179.89 (17)	N3′—C7′—C8′—C9′	171.82 (18)
O1—C8—C9—C14	115.0 (2)	O1′—C8′—C9′—C14′	116.4 (2)
C7—C8—C9—C14	−124.9 (2)	C7′—C8′—C9′—C14′	−123.2 (2)
O1—C8—C9—C10	−65.3 (2)	O1′—C8′—C9′—C10′	−64.3 (3)
C7—C8—C9—C10	54.9 (3)	C7′—C8′—C9′—C10′	56.1 (3)
C14—C9—C10—C11	0.8 (3)	C14′—C9′—C10′—C11′	0.0 (3)
C8—C9—C10—C11	−178.91 (19)	C8′—C9′—C10′—C11′	−179.3 (2)
C9—C10—C11—C12	−1.1 (3)	C9′—C10′—C11′—C12′	−0.6 (3)
C10—C11—C12—C13	0.4 (3)	C10′—C11′—C12′—C13′	0.6 (3)
C11—C12—C13—C14	0.6 (3)	C11′—C12′—C13′—C14′	0.1 (3)
C10—C9—C14—C13	0.1 (3)	C10′—C9′—C14′—C13′	0.7 (3)
C8—C9—C14—C13	179.87 (19)	C8′—C9′—C14′—C13′	179.99 (19)
C12—C13—C14—C9	−0.8 (3)	C12′—C13′—C14′—C9′	−0.8 (3)
C8—O1—C15—C16	−165.84 (19)	C8′—O1′—C15′—C16′	−154.90 (18)
O1—C15—C16—C21	−121.1 (2)	O1′—C15′—C16′—C17′	−124.1 (2)
O1—C15—C16—C17	59.8 (3)	O1′—C15′—C16′—C21′	55.9 (3)
C21—C16—C17—C18	0.9 (3)	C21′—C16′—C17′—C18′	−0.8 (3)
C15—C16—C17—C18	180.0 (2)	C15′—C16′—C17′—C18′	179.2 (2)
C16—C17—C18—C19	−1.3 (4)	C16′—C17′—C18′—C19′	0.5 (3)
C17—C18—C19—C20	1.2 (4)	C17′—C18′—C19′—C20′	0.1 (3)
C17—C18—C19—Cl1	−178.19 (18)	C17′—C18′—C19′—Cl1′	178.37 (17)
C18—C19—C20—C21	−0.8 (4)	C18′—C19′—C20′—C21′	−0.3 (4)
Cl1—C19—C20—C21	178.61 (17)	Cl1′—C19′—C20′—C21′	−178.62 (18)
C17—C16—C21—C20	−0.5 (3)	C19′—C20′—C21′—C16′	0.0 (4)
C15—C16—C21—C20	−179.5 (2)	C17′—C16′—C21′—C20′	0.5 (3)
C19—C20—C21—C16	0.4 (3)	C15′—C16′—C21′—C20′	−179.5 (2)

Hydrogen-bond geometry (Å, º)

Cg1, Cg2 and Cg3 are centroids of the C9–C14, C9′–C14′ and C16–C21 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11···*Cg*2^{i}	0.95	2.62	3.515 (2)	157
C11′—H11′···*Cg*1^{ii}	0.95	2.79	3.635 (2)	149
C14—H14···*Cg*2^{iii}	0.95	2.64	3.584 (2)	172

C14′—H14′···*Cg*1^{iv}	0.95	2.81	3.755 (2)	172
C18′—H18′···*Cg*3^{v}	0.95	2.83	3.502 (2)	129

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