

Crystal structure of 2-[2-(2,5-dichlorobenzoyloxy)-2-(furan-2-yl)ethyl]-2*H*-indazole

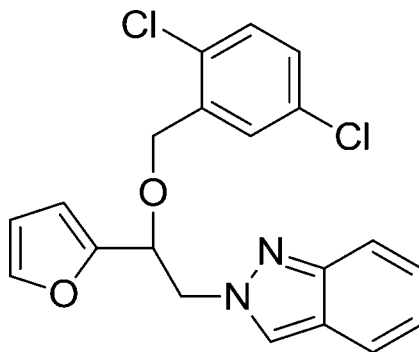
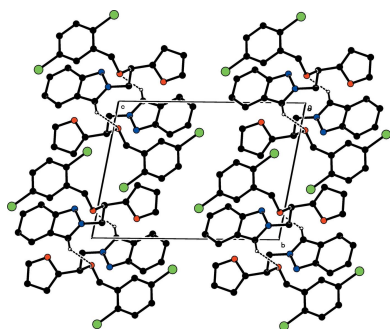
Özden Özel Güven,^a Gökhan Türk,^a Philip D. F. Adler,^b Simon J. Coles^b and Tuncer Hökelek^{c*}

^aDepartment of Chemistry, Bülent Ecevit University, 67100 Zonguldak, Turkey, ^bDepartment of Chemistry, Southampton University, SO17 1BJ Southampton, England, and ^cDepartment of Physics, Hacettepe University, 06800 Beytepe, Ankara, Turkey. *Correspondence e-mail: merzifon@hacettepe.edu.tr

In the title compound, C₂₀H₁₆Cl₂N₂O₂, the indazole ring system is approximately planar [maximum deviation = 0.033 (1) Å], its mean plane is oriented at dihedral angles of 25.04 (4) and 5.10 (4)° to the furan and benzene rings, respectively. In the crystal, pairs of C—H_{ind}···O_{bo} (ind = indazole and bo = benzyloxy) hydrogen bonds link the molecules into centrosymmetric dimers with graph-set motif $R_2^2(12)$. Weak C—H··· π interactions is also observed. Aromatic π – π stacking between the benzene and the pyrazole rings from neighbouring molecules [centroid–centroid distance = 3.8894 (7) Å] further consolidates the crystal packing.

1. Chemical context

Ethers such as miconazole and econazole possessing an imidazole ring have been developed for clinical uses as azole antifungals (Godefroi *et al.*, 1969). The crystal structures of miconazole (Peeters *et al.*, 1979) and econazole (Freer *et al.*, 1986) have previously been reported. Another azole ring system, indazole, is an important structural unit of many biologically active compounds. Some indazole derivatives have been shown to exhibit antifungal (Lebouvier *et al.*, 2007; Park *et al.*, 2007), antibacterial (Wang *et al.*, 2015), anti-proliferative (Büchel *et al.*, 2012), antitumor (Abbassi *et al.*, 2014) activity and act as inhibitors of nitric oxide synthase with antioxidant properties (Salerno *et al.*, 2012). The crystal structures of some indazole derivatives have been reported (Gerpe *et al.*, 2007; Raffa *et al.*, 2009; Boulhaoua *et al.*, 2015). In addition, the crystal structures of ketones containing an indazole group (Özel Güven *et al.*, 2013, 2014a) and ether (Özel Güven *et al.*, 2014b) have been described. As a continuation of our studies in this area, we synthesized the title compound and report herein its crystal structure.



2. Structural commentary

In the molecule of the title compound, (Fig. 1), the bond lengths and angles are within normal ranges. The indazole (*B*; N1/N2/C7–C13) ring system is approximately planar with a maximum deviation of -0.033 (1) Å for atom C10. Its mean plane is oriented with respect to the furan (*A*; O2/C2–C5) and benzene (*C*; C15–C20) rings at dihedral angles of $A/B = 25.04$ (4) and $B/C = 5.10$ (4)°. The dihedral angle between the furan and benzene rings is 20.21 (5)°. Atom C6 is -0.054 (1) Å from the indazole ring plane, while atom C1 is 0.038 (1) Å from the furan ring plane. Atoms C11, C12 and C14 are displaced by -0.0430 (3), 0.0233 (4) and -0.016 (1) Å, respectively, to the benzene ring plane.

3. Supramolecular features

In the crystal, pairs of $C-H_{\text{ind}} \cdots O_{\text{bo}}$ (ind = indazole and bo = benzyloxy) hydrogen bonds (Table 1), enclosing $R_2^2(12)$ ring motifs link the molecules into centrosymmetric dimers (Fig. 2), which are stacked along the *a* axis and oriented along the *b*-axis direction (Fig. 3). Weak $C-H \cdots \pi$ interactions (Table 1) occur. $\pi-\pi$ interactions between the pyrazole and the benzene rings, $Cg4 \cdots Cg3^i$, of neighbouring molecules further consolidate the crystal packing [centroid-centroid distance = 3.8894 (7) Å; symmetry code: (i) $2 - x, 2 - y, -z$; *Cg3* and *Cg4* are the centroids of rings *C* (C15–C20) and *D* (N1/N2/C7/C8/C13)].

4. Synthesis and crystallization

The title compound was synthesized by the reaction of 1-(furan-2-yl)-2-(2*H*-indazol-2-yl)ethanol with NaH and 2,5-dichlorobenzyl bromide. NaH (16 mg, 0.394 mmol) was added in small fractions to a solution of alcohol (90 mg, 0.394 mmol) in DMF (3–4 ml). Then, 2,5-dichlorobenzyl bromide (95 mg, 0.394 mmol) was added portionwise. The mixture was stirred at room temperature for 3 h, and the excess hydride was decomposed with a small amount of methyl alcohol. After evaporation to dryness under reduced pressure, a small amount of water was added and extracted with methylene

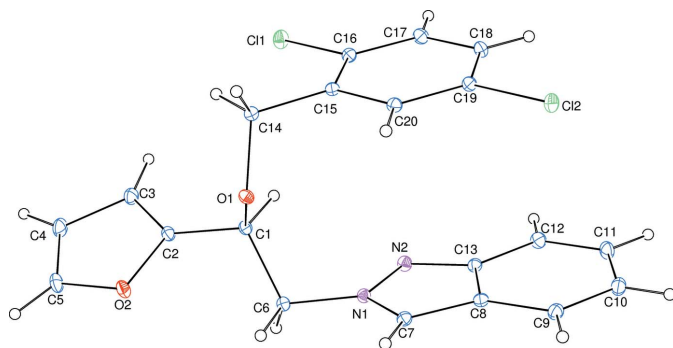


Figure 1
The molecular structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

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

Cg4 is the centroid of the N1/N2/C7/C8/C13 ring.

<i>D</i> –H \cdots <i>A</i>	<i>D</i> –H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> –H \cdots <i>A</i>
C7–H7 \cdots O1 ⁱ	0.93	2.51	3.3062 (15)	144
C6–H6B \cdots Cg4 ⁱⁱ	0.97	2.84	3.4583 (13)	122

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

chloride. The organic layer was separated, dried over anhydrous sodium sulfate, and then evaporated to dryness. The crude residue was purified by chromatography on a silica-gel column using a hexane–ethyl acetate mixture (10:1) as eluent. The ether was recrystallized from 2-propanol solution to obtain colourless crystals suitable for X-ray analysis (yield; 70 mg, 46%).

5. Refinement

The experimental details including the crystal data, data collection and refinement are summarized in Table 2. The C-bound H atoms were positioned geometrically with $C-H = 0.93, 0.97$ and 0.98 Å, for aromatic, methylene and methine H-atoms, respectively, and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

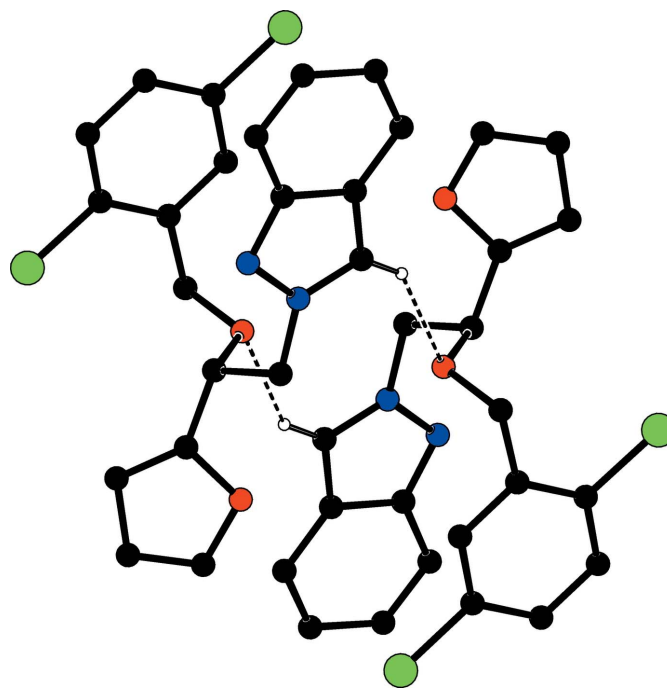


Figure 2
Part of the crystal structure. Intermolecular $[C-H_{\text{ind}} \cdots O_{\text{bo}}]$ hydrogen bonds, enclosing $R_2^2(12)$ ring motifs, are shown as dashed lines (see Table 1). H atoms not involved in hydrogen bonding have been omitted for clarity.

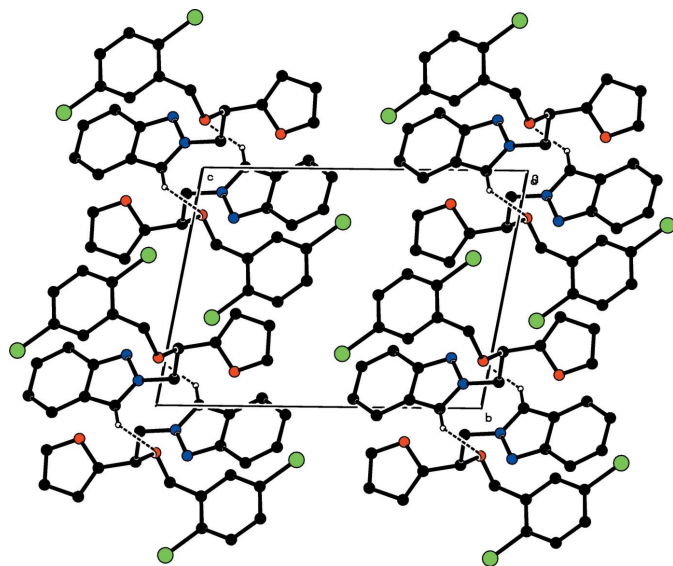


Figure 3
The crystal packing of the title compound, viewed down the *a* axis. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity.

Acknowledgements

The authors acknowledge the Zonguldak Karaelmas University Research Fund (project No. 2012-10-03-12) for support.

References

Abbassi, N., Rakib, E. M., Chicha, H., Bouissane, L., Hannioui, A., Aiello, C., Gangemi, R., Castagnola, P., Rosano, C. & Viale, M. (2014). *Arch. Pharm. Chem. Life Sci.* **347**, 423–431.
 Boulhaoua, M., Benchidmi, M., Essassi, E. M., Saadi, M. & El Ammari, L. (2015). *Acta Cryst.* **E71**, o780–o781.
 Büchel, G. E., Stepanenko, I. N., Hejl, M., Jakupec, M. A., Keppler, B. K., Heffeter, P., Berger, W. & Arion, V. B. (2012). *J. Inorg. Biochem.* **113**, 47–54.
 Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
 Freer, A. A., Pearson, A. & Salole, E. G. (1986). *Acta Cryst.* **C42**, 1350–1352.
 Gerpe, A., Piro, O. E., Cerecetto, H. & González, M. (2007). *J. Mol. Struct.* **871**, 98–107.
 Godefroi, E. F., Heeres, J., Van Cutsem, J. & Janssen, P. A. (1969). *J. Med. Chem.* **12**, 784–791.
 Lebouvier, N., Pagniez, F., Dufflos, M., Le Pape, P., Na, Y. M., Le Baut, G. & Le Borgne, M. (2007). *Bioorg. Med. Chem. Lett.* **17**, 3686–3689.
 Özel Güven, Ö., Türk, G., Adler, P. D. F., Coles, S. J. & Hökelek, T. (2013). *Acta Cryst.* **E69**, o184.

Table 2
Experimental details.

Crystal data	
Chemical formula	C ₂₀ H ₁₆ Cl ₂ N ₂ O ₂
<i>M_r</i>	387.27
Crystal system, space group	Triclinic, <i>P</i> $\bar{1}$
Temperature (K)	294
<i>a</i> , <i>b</i> , <i>c</i> (Å)	7.7318 (3), 9.6675 (4), 12.8299 (5)
α , β , γ (°)	76.511 (4), 76.157 (4), 73.928 (3)
<i>V</i> (Å ³)	880.30 (6)
<i>Z</i>	2
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.39
Crystal size (mm)	0.09 × 0.07 × 0.04
Data collection	
Diffractometer	Rigaku Saturn724+
Absorption correction	Multi-scan (<i>CrystalClear-SM Expert</i> , Rigaku, 2011)
<i>T_{min}</i> , <i>T_{max}</i>	0.968, 0.985
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	8400, 4278, 3813
<i>R_{int}</i>	0.025
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.674
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.031, 0.083, 1.05
No. of reflections	4278
No. of parameters	235
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å ⁻³)	0.35, -0.23

Computer programs: *CrystalClear-SM Expert* (Rigaku, 2011), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

Özel Güven, Ö., Türk, G., Adler, P. D. F., Coles, S. J. & Hökelek, T. (2014a). *Acta Cryst.* **E70**, o505.
 Özel Güven, Ö., Türk, G., Adler, P. D. F., Coles, S. J. & Hökelek, T. (2014b). *Acta Cryst.* **E70**, o410.
 Park, J. S., Yu, K. A., Kang, T. H., Kim, S. & Suh, Y. G. (2007). *Bioorg. Med. Chem. Lett.* **17**, 3486–3490.
 Peeters, O. M., Blaton, N. M. & De Ranter, C. J. (1979). *Acta Cryst.* **B35**, 2461–2464.
 Raffa, D., Maggio, B., Cascioferro, S., Raimondi, M. V., Schillaci, D., Gallo, G., Daidone, G., Plescia, S., Meneghetti, F., Bombieri, G., Di Cristina, A., Pipitone, R. M., Grimaudo, S. & Tolomeo, M. (2009). *Eur. J. Med. Chem.* **44**, 165–178.
 Rigaku (2011). *CrystalClear*, Rigaku Corporation, Tokyo, Japan.
 Salerno, L., Modica, M. N., Romeo, G., Pittalà, V., Siracusa, M. A., Amato, M. E., Acquaviva, R., Di Giacomo, C. & Sorrenti, V. (2012). *Eur. J. Med. Chem.* **49**, 118–126.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
 Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.
 Wang, Y., Yan, M., Ma, R. & Ma, S. (2015). *Arch. Pharm. Chem. Life Sci.* **348**, 266–274.

supporting information

Acta Cryst. (2016). E72, 1377-1379 [https://doi.org/10.1107/S2056989016013827]

Crystal structure of 2-[2-(2,5-dichlorobenzyloxy)-2-(furan-2-yl)ethyl]-2H-indazole

Özden Özel Güven, Gökhan Türk, Philip D. F. Adler, Simon J. Coles and Tuncer Hökelek

Computing details

Data collection: *CrystalClear-SM Expert* (Rigaku, 2011); cell refinement: *CrystalClear-SM Expert* (Rigaku, 2011); data reduction: *CrystalClear-SM Expert* (Rigaku, 2011); 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); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

2-[2-(2,5-Dichlorobenzyloxy)-2-(furan-2-yl)ethyl]-2H-indazole

Crystal data

$C_{20}H_{16}Cl_2N_2O_2$
 $M_r = 387.27$
 Triclinic, *P1*
 Hall symbol: -P 1
 $a = 7.7318$ (3) Å
 $b = 9.6675$ (4) Å
 $c = 12.8299$ (5) Å
 $\alpha = 76.511$ (4)°
 $\beta = 76.157$ (4)°
 $\gamma = 73.928$ (3)°
 $V = 880.30$ (6) Å³

$Z = 2$
 $F(000) = 400$
 $D_x = 1.461$ Mg m⁻³
 Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
 Cell parameters from 7516 reflections
 $\theta = 3.0$ – 28.6 °
 $\mu = 0.39$ mm⁻¹
 $T = 294$ K
 Block, colorless
 $0.09 \times 0.07 \times 0.04$ mm

Data collection

Rigaku Saturn724+
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 ω scans
 Absorption correction: multi-scan
 (*CrystalClear-SM Expert*, Rigaku, 2011)
 $T_{\min} = 0.968$, $T_{\max} = 0.985$
 8400 measured reflections

4278 independent reflections
 3813 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.025$
 $\theta_{\max} = 28.6$ °, $\theta_{\min} = 3.0$ °
 $h = -6 \rightarrow 10$
 $k = -13 \rightarrow 13$
 $l = -17 \rightarrow 17$
 3 standard reflections every 120 min
 intensity decay: 1%

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.031$
 $wR(F^2) = 0.083$
 $S = 1.05$
 4278 reflections
 235 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
 $w = 1/[\sigma^2(F_o^2) + (0.0387P)^2 + 0.3381P]$
 where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.35 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.23 \text{ e } \text{\AA}^{-3}$

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 $F^2 > 2\text{sigma}(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl1	0.24682 (4)	0.62858 (3)	0.88313 (3)	0.02337 (9)
Cl2	0.49082 (5)	0.22144 (3)	0.53654 (2)	0.02445 (9)
O1	0.44963 (11)	0.19772 (8)	0.97438 (7)	0.01525 (17)
O2	0.31136 (12)	0.14245 (9)	1.21688 (7)	0.02059 (19)
N1	0.15767 (13)	0.10240 (10)	0.92745 (8)	0.01489 (19)
N2	0.03507 (13)	0.21036 (11)	0.87622 (8)	0.0175 (2)
C1	0.26260 (15)	0.23752 (12)	1.03067 (9)	0.0143 (2)
H1	0.1970	0.3262	0.9884	0.017*
C2	0.25595 (15)	0.26448 (13)	1.14153 (9)	0.0161 (2)
C3	0.21044 (18)	0.38619 (14)	1.18630 (10)	0.0211 (2)
H3	0.1687	0.4820	1.1524	0.025*
C4	0.23944 (19)	0.33774 (15)	1.29692 (11)	0.0254 (3)
H4	0.2204	0.3962	1.3487	0.031*
C5	0.29944 (18)	0.19136 (15)	1.31093 (10)	0.0236 (3)
H5	0.3288	0.1316	1.3755	0.028*
C6	0.17821 (16)	0.11038 (12)	1.03596 (9)	0.0160 (2)
H6A	0.2559	0.0195	1.0659	0.019*
H6B	0.0592	0.1233	1.0839	0.019*
C7	0.25036 (15)	-0.00406 (12)	0.87016 (10)	0.0156 (2)
H7	0.3402	-0.0856	0.8913	0.019*
C8	0.18475 (15)	0.03232 (12)	0.77239 (10)	0.0156 (2)
C9	0.21674 (17)	-0.03471 (13)	0.68025 (10)	0.0188 (2)
H9	0.3022	-0.1232	0.6750	0.023*
C10	0.11867 (17)	0.03397 (14)	0.59908 (10)	0.0214 (2)
H10	0.1362	-0.0095	0.5387	0.026*
C11	-0.00995 (17)	0.17116 (14)	0.60570 (10)	0.0222 (3)
H11	-0.0724	0.2161	0.5485	0.027*
C12	-0.04425 (17)	0.23857 (13)	0.69382 (10)	0.0203 (2)
H12	-0.1283	0.3281	0.6970	0.024*
C13	0.05251 (15)	0.16753 (12)	0.78018 (9)	0.0158 (2)
C14	0.51911 (16)	0.32122 (12)	0.91196 (9)	0.0157 (2)
H14A	0.6518	0.2928	0.8940	0.019*

H14B	0.4856	0.3981	0.9550	0.019*
C15	0.44190 (15)	0.37805 (12)	0.80800 (9)	0.0149 (2)
C16	0.32003 (16)	0.51321 (12)	0.78692 (10)	0.0169 (2)
C17	0.24998 (17)	0.55987 (13)	0.69043 (10)	0.0204 (2)
H17	0.1687	0.6505	0.6783	0.024*
C18	0.30253 (17)	0.47018 (14)	0.61306 (10)	0.0210 (2)
H18	0.2581	0.5002	0.5482	0.025*
C19	0.42271 (16)	0.33464 (13)	0.63373 (10)	0.0180 (2)
C20	0.49107 (16)	0.28785 (13)	0.72976 (9)	0.0166 (2)
H20	0.5699	0.1961	0.7422	0.020*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.02851 (16)	0.01783 (14)	0.02403 (16)	0.00089 (11)	-0.00838 (12)	-0.00825 (11)
Cl2	0.03293 (17)	0.02802 (16)	0.01613 (15)	-0.01132 (13)	-0.00224 (12)	-0.00855 (11)
O1	0.0145 (4)	0.0151 (4)	0.0142 (4)	-0.0024 (3)	-0.0014 (3)	-0.0015 (3)
O2	0.0261 (4)	0.0211 (4)	0.0132 (4)	-0.0024 (3)	-0.0051 (3)	-0.0027 (3)
N1	0.0148 (4)	0.0151 (4)	0.0151 (5)	-0.0031 (3)	-0.0037 (4)	-0.0026 (3)
N2	0.0166 (5)	0.0168 (5)	0.0189 (5)	-0.0014 (4)	-0.0057 (4)	-0.0032 (4)
C1	0.0144 (5)	0.0148 (5)	0.0129 (5)	-0.0022 (4)	-0.0021 (4)	-0.0026 (4)
C2	0.0151 (5)	0.0191 (5)	0.0135 (5)	-0.0041 (4)	-0.0026 (4)	-0.0016 (4)
C3	0.0253 (6)	0.0211 (6)	0.0184 (6)	-0.0050 (5)	-0.0049 (5)	-0.0060 (4)
C4	0.0312 (7)	0.0310 (7)	0.0177 (6)	-0.0082 (5)	-0.0044 (5)	-0.0105 (5)
C5	0.0263 (6)	0.0324 (7)	0.0125 (5)	-0.0060 (5)	-0.0049 (5)	-0.0045 (5)
C6	0.0182 (5)	0.0168 (5)	0.0134 (5)	-0.0049 (4)	-0.0028 (4)	-0.0027 (4)
C7	0.0152 (5)	0.0146 (5)	0.0172 (5)	-0.0032 (4)	-0.0032 (4)	-0.0033 (4)
C8	0.0143 (5)	0.0159 (5)	0.0169 (5)	-0.0053 (4)	-0.0020 (4)	-0.0023 (4)
C9	0.0196 (5)	0.0195 (5)	0.0187 (6)	-0.0059 (4)	-0.0021 (4)	-0.0058 (4)
C10	0.0222 (6)	0.0268 (6)	0.0183 (6)	-0.0083 (5)	-0.0034 (5)	-0.0071 (5)
C11	0.0225 (6)	0.0273 (6)	0.0187 (6)	-0.0061 (5)	-0.0093 (5)	-0.0018 (5)
C12	0.0186 (5)	0.0201 (6)	0.0219 (6)	-0.0027 (4)	-0.0067 (5)	-0.0026 (5)
C13	0.0150 (5)	0.0168 (5)	0.0163 (5)	-0.0050 (4)	-0.0025 (4)	-0.0030 (4)
C14	0.0158 (5)	0.0163 (5)	0.0154 (5)	-0.0047 (4)	-0.0030 (4)	-0.0024 (4)
C15	0.0143 (5)	0.0164 (5)	0.0148 (5)	-0.0058 (4)	-0.0021 (4)	-0.0022 (4)
C16	0.0186 (5)	0.0158 (5)	0.0167 (5)	-0.0046 (4)	-0.0032 (4)	-0.0034 (4)
C17	0.0225 (6)	0.0180 (5)	0.0201 (6)	-0.0039 (4)	-0.0075 (5)	0.0000 (4)
C18	0.0251 (6)	0.0246 (6)	0.0149 (5)	-0.0093 (5)	-0.0069 (5)	0.0009 (4)
C19	0.0201 (5)	0.0216 (6)	0.0140 (5)	-0.0094 (5)	-0.0004 (4)	-0.0042 (4)
C20	0.0169 (5)	0.0169 (5)	0.0161 (5)	-0.0053 (4)	-0.0020 (4)	-0.0026 (4)

Geometric parameters (Å, °)

Cl1—C16	1.7453 (12)	C8—C13	1.4269 (16)
Cl2—C19	1.7416 (12)	C9—C8	1.4169 (17)
O1—C1	1.4431 (13)	C9—C10	1.3699 (17)
O1—C14	1.4348 (13)	C9—H9	0.9300
O2—C2	1.3770 (14)	C10—C11	1.4272 (18)

O2—C5	1.3701 (15)	C10—H10	0.9300
N1—C6	1.4601 (14)	C11—H11	0.9300
N1—C7	1.3437 (15)	C12—C11	1.3703 (18)
N2—N1	1.3603 (13)	C12—C13	1.4199 (16)
N2—C13	1.3548 (15)	C12—H12	0.9300
C1—C6	1.5248 (15)	C14—H14A	0.9700
C1—H1	0.9800	C14—H14B	0.9700
C2—C1	1.4913 (16)	C15—C14	1.5149 (15)
C2—C3	1.3519 (17)	C15—C16	1.3942 (16)
C3—C4	1.4380 (17)	C15—C20	1.3981 (16)
C3—H3	0.9300	C16—C17	1.3980 (16)
C4—H4	0.9300	C17—H17	0.9300
C5—C4	1.3445 (19)	C18—C17	1.3841 (18)
C5—H5	0.9300	C18—C19	1.3901 (18)
C6—H6A	0.9700	C18—H18	0.9300
C6—H6B	0.9700	C19—C20	1.3861 (16)
C7—H7	0.9300	C20—H20	0.9300
C8—C7	1.3980 (16)		
C14—O1—C1	113.25 (8)	C10—C9—H9	120.8
C5—O2—C2	106.39 (10)	C9—C10—C11	121.05 (12)
N2—N1—C6	119.34 (9)	C9—C10—H10	119.5
C7—N1—N2	114.58 (10)	C11—C10—H10	119.5
C7—N1—C6	126.08 (10)	C10—C11—H11	119.0
C13—N2—N1	103.16 (9)	C12—C11—C10	121.96 (11)
O1—C1—C2	110.75 (9)	C12—C11—H11	119.0
O1—C1—C6	105.96 (9)	C11—C12—C13	117.94 (11)
O1—C1—H1	109.4	C11—C12—H12	121.0
C2—C1—C6	111.85 (9)	C13—C12—H12	121.0
C2—C1—H1	109.4	N2—C13—C8	111.76 (10)
C6—C1—H1	109.4	N2—C13—C12	128.06 (11)
O2—C2—C1	115.82 (10)	C12—C13—C8	120.17 (11)
C3—C2—O2	110.25 (10)	O1—C14—C15	110.37 (9)
C3—C2—C1	133.91 (11)	O1—C14—H14A	109.6
C2—C3—C4	106.19 (11)	O1—C14—H14B	109.6
C2—C3—H3	126.9	C15—C14—H14A	109.6
C4—C3—H3	126.9	C15—C14—H14B	109.6
C3—C4—H4	126.7	H14A—C14—H14B	108.1
C5—C4—C3	106.63 (11)	C16—C15—C14	123.97 (10)
C5—C4—H4	126.7	C16—C15—C20	117.85 (11)
O2—C5—H5	124.7	C20—C15—C14	118.16 (10)
C4—C5—O2	110.55 (11)	C15—C16—C11	120.24 (9)
C4—C5—H5	124.7	C15—C16—C17	121.87 (11)
N1—C6—C1	110.63 (9)	C17—C16—C11	117.87 (9)
N1—C6—H6A	109.5	C16—C17—H17	120.3
N1—C6—H6B	109.5	C18—C17—C16	119.50 (11)
C1—C6—H6A	109.5	C18—C17—H17	120.3
C1—C6—H6B	109.5	C17—C18—C19	119.07 (11)

H6A—C6—H6B	108.1	C17—C18—H18	120.5
N1—C7—C8	106.25 (10)	C19—C18—H18	120.5
N1—C7—H7	126.9	C18—C19—C12	119.43 (9)
C8—C7—H7	126.9	C20—C19—C12	119.11 (9)
C7—C8—C9	135.24 (11)	C20—C19—C18	121.45 (11)
C7—C8—C13	104.23 (10)	C15—C20—H20	119.9
C9—C8—C13	120.48 (11)	C19—C20—C15	120.25 (11)
C8—C9—H9	120.8	C19—C20—H20	119.9
C10—C9—C8	118.36 (11)		
C14—O1—C1—C2	-89.83 (11)	C7—C8—C13—N2	-1.03 (13)
C14—O1—C1—C6	148.69 (9)	C7—C8—C13—C12	-179.97 (10)
C1—O1—C14—C15	-75.87 (11)	C9—C8—C13—N2	176.94 (10)
C5—O2—C2—C1	178.44 (10)	C9—C8—C13—C12	-2.01 (17)
C5—O2—C2—C3	-0.06 (13)	C10—C9—C8—C7	177.63 (13)
C2—O2—C5—C4	-0.05 (14)	C10—C9—C8—C13	0.43 (17)
N2—N1—C6—C1	-67.74 (13)	C8—C9—C10—C11	1.28 (18)
C7—N1—C6—C1	112.18 (12)	C9—C10—C11—C12	-1.5 (2)
N2—N1—C7—C8	-0.85 (13)	C13—C12—C11—C10	-0.12 (19)
C6—N1—C7—C8	179.22 (10)	C11—C12—C13—N2	-176.94 (12)
C13—N2—N1—C6	-179.86 (10)	C11—C12—C13—C8	1.81 (17)
C13—N2—N1—C7	0.21 (13)	C16—C15—C14—O1	112.32 (12)
N1—N2—C13—C8	0.53 (12)	C20—C15—C14—O1	-65.60 (13)
N1—N2—C13—C12	179.37 (11)	C14—C15—C16—C11	-0.09 (16)
O1—C1—C6—N1	-69.01 (11)	C14—C15—C16—C17	-178.88 (11)
C2—C1—C6—N1	170.22 (9)	C20—C15—C16—C11	177.83 (9)
O2—C2—C1—O1	-71.29 (12)	C20—C15—C16—C17	-0.95 (17)
O2—C2—C1—C6	46.66 (13)	C14—C15—C20—C19	179.49 (10)
C3—C2—C1—O1	106.75 (15)	C16—C15—C20—C19	1.44 (17)
C3—C2—C1—C6	-135.30 (14)	C11—C16—C17—C18	-178.91 (9)
O2—C2—C3—C4	0.13 (14)	C15—C16—C17—C18	-0.10 (19)
C1—C2—C3—C4	-177.99 (13)	C19—C18—C17—C16	0.66 (18)
C2—C3—C4—C5	-0.16 (15)	C17—C18—C19—C12	-179.60 (9)
O2—C5—C4—C3	0.13 (16)	C17—C18—C19—C20	-0.16 (18)
C9—C8—C7—N1	-176.43 (13)	C12—C19—C20—C15	178.52 (9)
C13—C8—C7—N1	1.08 (12)	C18—C19—C20—C15	-0.92 (18)

Hydrogen-bond geometry (Å, °)

Cg4 is the centroid of the N1/N2/C7/C8/C13 ring.

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C7—H7 \cdots O1 ⁱ	0.93	2.51	3.3062 (15)	144
C6—H6B \cdots Cg4 ⁱⁱ	0.97	2.84	3.4583 (13)	122

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