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Ethyl 1-benzyl-2-(3-chlorophenyl)-1*H*-benzimidazole-5-carboxylate

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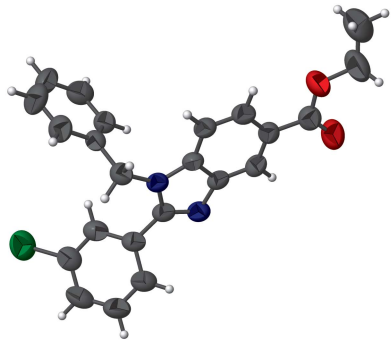
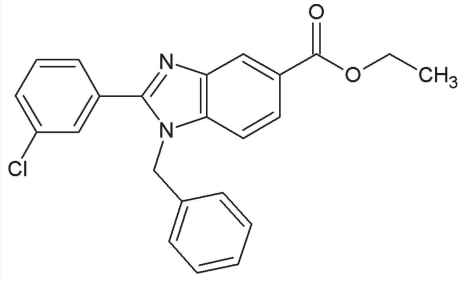
In the title compound, $C_{23}H_{19}ClN_2O_2$, the dihedral angles between the imidazole ring system and the chlorobenzene and phenyl rings are 48.05 (14) and 82.53 (15)°, respectively. In the crystal, inversion dimers linked by pairs of C—H···O hydrogen bonds generate $R_2^2(22)$ loops. Weak C—H···π and π–π stacking interactions are also observed.

3D view



Chemical scheme



Structure description

As part of our research on the synthesis and crystal structures of 1,2-disubstituted benzimidazole-5-carboxylates, we report here the crystal and molecular structure of ethyl 1-benzyl-2-(3-chlorophenyl)-1*H*-benzimidazole-5-carboxylate, (I). The molecular structure of (I) is shown in Fig. 1 and the dihedral angle between the chlorobenzene (C11–C16) and phenyl (C1–C6) rings is 74.06 (18)°.

In the crystal (Fig. 2), molecules are linked into inversion dimers through pairs of C1—H1···O2 hydrogen bonds, forming an $R_2^2(22)$ loop (Table 1) and a weak C—H···π bond is observed. Aromatic π–π stacking, with a centroid–centroid distance of 3.866 (2) Å [$Cg1\cdots Cg2$, where $Cg1$ and $Cg2(-x+2, y+\frac{1}{2}, -z+\frac{1}{2})$ are the centroids of rings N1/C8/C9/N2/C10 and C1–C6, respectively], also occurs.

Synthesis and crystallization

Sodium dithionite (3.0 equivalents) was added to a stirred solution of ethyl 4-benzylamino-3-nitrobenzoate (0.01 mol, 1.0 equivalent) and 3-chlorobenzaldehyde (0.01 mol, 1.0 equivalent) in DMSO (20 ml). The reaction mixture was stirred at 363 K for 3 h. After

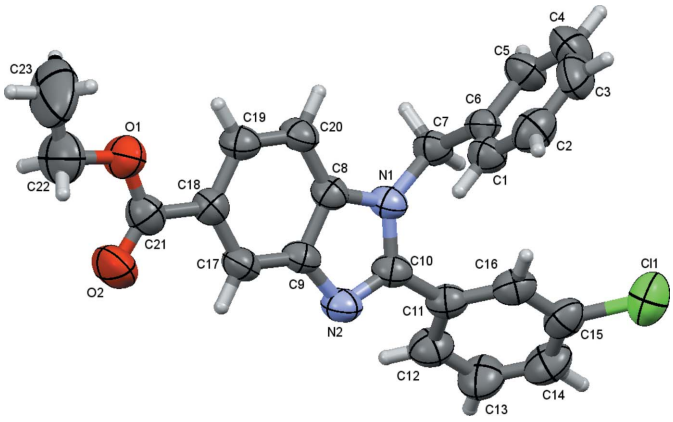


Figure 1
The molecular structure of (I), showing 50% displacement ellipsods.

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

*Cg*4 is the centroid of the C11–C16 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···O2^{i}	0.93	2.54	3.358 (4)	148
C20—H20···*Cg*4^{ii}	0.93	2.87	3.757 (4)	159

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

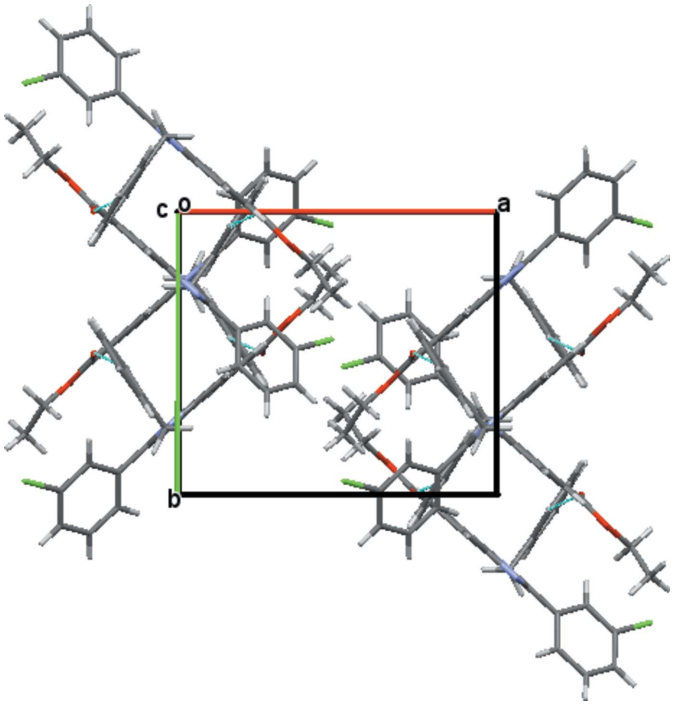


Figure 2
The packing of (I), viewed down [001].

completion of the reaction (monitored by TLC; hexane–ethyl acetate 7:3 *v*/*v*), it was poured onto crushed ice. The solid separated was filtered off, washed with water and dried. The product was recrystallized from *N*,*N*-dimethyformamide solution to yield colourless blocks.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{23}H_{19}ClN_2O_2$
M_r	390.85
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	11.145 (3), 9.878 (2), 18.355 (4)
β (°)	93.952 (7)
V (Å^3)	2015.9 (8)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.21
Crystal size (mm)	0.32 × 0.26 × 0.21
Data collection	
Diffractometer	Rigaku Saturn724+
Absorption correction	Multi-scan (*NUMABS*; Rigaku 1999)
T_{min}, T_{max}	0.935, 0.957
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14125, 4498, 2287
R_{int}	0.048
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.649
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.078, 0.185, 1.04
No. of reflections	4498
No. of parameters	254
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.22, −0.29

Computer programs: *CrystalClear SM Expert* (Rigaku, 2011), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *Mercury* (Macrae *et al.*, 2008) and *OLEX2* (Dolomanov *et al.*, 2009).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

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Crystal data

$C_{23}H_{19}ClN_2O_2$
M_r = 390.85
Monoclinic, $P2_1/c$
a = 11.145 (3) Å
b = 9.878 (2) Å
c = 18.355 (4) Å
β = 93.952 (7)°
V = 2015.9 (8) Å^3
Z = 4
$F(000)$ = 816
D_x = 1.288 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71075 Å
Cell parameters from 4498 reflections
θ = 3.0–27.5°
μ = 0.21 mm^{-1}
T = 296 K
Block, colourless
0.32 × 0.26 × 0.21 mm

Data collection

Rigaku Saturn724+ diffractometer
profile data from ω–scans
Absorption correction: multi-scan (NUMABS; Rigaku 1999)
T_{min} = 0.935, T_{max} = 0.957
14125 measured reflections
4498 independent reflections
2287 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
θ_{max} = 27.5°, θ_{min} = 3.0°
h = −14→14
k = −12→12
l = −23→23
4498 standard reflections

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.078
$wR(F^2)$ = 0.185
S = 1.04
4498 reflections
254 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0581P)^2 + 1.0114P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.51971 (9)	0.95208 (12)	0.21673 (7)	0.1007 (4)
O1	1.3420 (2)	0.3900 (3)	0.50007 (13)	0.0834 (8)
N1	0.9704 (2)	0.7556 (3)	0.32335 (13)	0.0537 (6)
C6	0.8897 (3)	0.6538 (3)	0.20635 (16)	0.0509 (8)
C9	1.0335 (3)	0.7003 (3)	0.43583 (16)	0.0534 (8)
C8	1.0530 (3)	0.6769 (3)	0.36265 (16)	0.0520 (8)
N2	0.9413 (2)	0.7933 (3)	0.44078 (15)	0.0626 (7)
C17	1.1037 (3)	0.6343 (3)	0.48961 (17)	0.0595 (8)
H17	1.0919	0.6482	0.5387	0.071*
C18	1.1919 (3)	0.5472 (3)	0.46873 (17)	0.0562 (8)
C7	0.9609 (3)	0.7653 (3)	0.24414 (16)	0.0585 (8)
H7A	1.0413	0.7652	0.2270	0.070*
H7B	0.9238	0.8512	0.2303	0.070*
C16	0.7209 (3)	0.8924 (3)	0.30033 (18)	0.0627 (9)
H16	0.7198	0.8098	0.2760	0.075*
C21	1.2678 (3)	0.4790 (4)	0.5267 (2)	0.0688 (10)
C11	0.8119 (3)	0.9214 (3)	0.35294 (18)	0.0582 (8)
C20	1.1417 (3)	0.5909 (3)	0.34119 (17)	0.0586 (8)
H20	1.1541	0.5770	0.2922	0.070*
C5	0.8807 (3)	0.6533 (4)	0.13092 (18)	0.0727 (10)
H5	0.9178	0.7216	0.1058	0.087*
O2	1.2644 (3)	0.5004 (3)	0.59070 (15)	0.1004 (10)
C10	0.9073 (3)	0.8236 (3)	0.37328 (18)	0.0555 (8)
C19	1.2099 (3)	0.5275 (3)	0.39501 (18)	0.0611 (9)
H19	1.2705	0.4691	0.3823	0.073*
C1	0.8341 (3)	0.5539 (3)	0.24296 (18)	0.0608 (9)
H1	0.8386	0.5532	0.2937	0.073*
C12	0.8114 (3)	1.0456 (3)	0.3880 (2)	0.0725 (10)
H12	0.8721	1.0665	0.4236	0.087*
C14	0.6328 (4)	1.1091 (4)	0.3193 (2)	0.0830 (12)
H14	0.5727	1.1725	0.3079	0.100*
C2	0.7709 (3)	0.4538 (4)	0.2039 (2)	0.0799 (11)
H2	0.7324	0.3858	0.2284	0.096*
C15	0.6316 (3)	0.9865 (4)	0.2840 (2)	0.0687 (10)
C3	0.7650 (4)	0.4553 (5)	0.1288 (3)	0.0900 (13)
H3	0.7239	0.3871	0.1026	0.108*
C4	0.8189 (4)	0.5554 (5)	0.0930 (2)	0.0959 (14)
H4	0.8135	0.5570	0.0422	0.115*
C13	0.7226 (4)	1.1370 (4)	0.3709 (2)	0.0867 (12)
H13	0.7235	1.2200	0.3949	0.104*
C22	1.4205 (4)	0.3153 (5)	0.5511 (2)	0.1122 (16)
H22A	1.4797	0.3756	0.5750	0.135*
H22B	1.3745	0.2742	0.5882	0.135*
C23	1.4792 (6)	0.2127 (7)	0.5113 (4)	0.184 (3)
H23A	1.5219	0.2542	0.4735	0.276*

H23B	1.4202	0.1511	0.4899	0.276*
H23C	1.5348	0.1642	0.5439	0.276*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0690 (6)	0.1118 (9)	0.1198 (10)	−0.0021 (6)	−0.0056 (6)	0.0058 (7)
O1	0.0883 (18)	0.0881 (18)	0.0733 (17)	0.0306 (15)	0.0018 (14)	0.0091 (14)
N1	0.0645 (16)	0.0493 (15)	0.0478 (15)	0.0035 (13)	0.0081 (13)	−0.0047 (12)
C6	0.0536 (17)	0.055 (2)	0.0442 (18)	0.0093 (15)	0.0078 (14)	0.0019 (15)
C9	0.0639 (19)	0.0501 (19)	0.0470 (19)	−0.0026 (16)	0.0088 (15)	−0.0090 (15)
C8	0.0611 (19)	0.0429 (18)	0.0520 (19)	0.0000 (15)	0.0041 (15)	−0.0054 (15)
N2	0.0725 (18)	0.0609 (18)	0.0551 (18)	0.0096 (14)	0.0101 (14)	−0.0090 (14)
C17	0.068 (2)	0.066 (2)	0.0446 (18)	−0.0028 (18)	0.0066 (16)	−0.0067 (16)
C18	0.0587 (19)	0.057 (2)	0.053 (2)	−0.0003 (16)	0.0030 (15)	−0.0002 (16)
C7	0.067 (2)	0.059 (2)	0.0499 (19)	0.0057 (17)	0.0119 (16)	0.0058 (16)
C16	0.066 (2)	0.053 (2)	0.071 (2)	−0.0004 (17)	0.0182 (18)	−0.0003 (17)
C21	0.075 (2)	0.070 (2)	0.061 (2)	−0.002 (2)	0.004 (2)	0.0052 (19)
C11	0.065 (2)	0.050 (2)	0.061 (2)	0.0029 (16)	0.0153 (17)	−0.0004 (16)
C20	0.072 (2)	0.057 (2)	0.0472 (19)	0.0066 (17)	0.0067 (16)	−0.0095 (16)
C5	0.082 (2)	0.088 (3)	0.049 (2)	0.003 (2)	0.0085 (18)	0.005 (2)
O2	0.118 (2)	0.128 (3)	0.0543 (17)	0.0326 (19)	−0.0011 (15)	0.0054 (16)
C10	0.066 (2)	0.0480 (19)	0.054 (2)	0.0010 (16)	0.0112 (16)	−0.0060 (16)
C19	0.068 (2)	0.057 (2)	0.059 (2)	0.0052 (17)	0.0108 (17)	−0.0074 (17)
C1	0.068 (2)	0.062 (2)	0.0523 (19)	0.0029 (18)	0.0063 (16)	0.0027 (17)
C12	0.078 (2)	0.059 (2)	0.081 (3)	0.0066 (19)	0.011 (2)	−0.008 (2)
C14	0.079 (3)	0.065 (3)	0.107 (3)	0.022 (2)	0.017 (2)	0.007 (2)
C2	0.069 (2)	0.070 (3)	0.101 (3)	−0.002 (2)	0.011 (2)	−0.001 (2)
C15	0.058 (2)	0.071 (3)	0.079 (2)	−0.0002 (18)	0.0146 (18)	0.009 (2)
C3	0.078 (3)	0.103 (4)	0.086 (3)	0.005 (2)	−0.021 (2)	−0.032 (3)
C4	0.106 (3)	0.123 (4)	0.057 (3)	−0.005 (3)	−0.007 (2)	−0.014 (3)
C13	0.089 (3)	0.064 (3)	0.107 (3)	0.017 (2)	0.003 (3)	−0.017 (2)
C22	0.119 (4)	0.121 (4)	0.095 (3)	0.039 (3)	−0.010 (3)	0.027 (3)
C23	0.165 (6)	0.183 (6)	0.194 (7)	0.103 (5)	−0.066 (5)	−0.041 (5)

Geometric parameters (Å, º)

Cl1—C15	1.728 (4)	C11—C12	1.386 (4)
O1—C21	1.324 (4)	C20—H20	0.9300
O1—C22	1.440 (4)	C20—C19	1.357 (4)
N1—C8	1.372 (4)	C5—H5	0.9300
N1—C7	1.454 (4)	C5—C4	1.352 (5)
N1—C10	1.369 (4)	C19—H19	0.9300
C6—C7	1.499 (4)	C1—H1	0.9300
C6—C5	1.381 (4)	C1—C2	1.385 (5)
C6—C1	1.367 (4)	C12—H12	0.9300
C9—C8	1.395 (4)	C12—C13	1.360 (5)
C9—N2	1.387 (4)	C14—H14	0.9300

C9—C17	1.380 (4)	C14—C15	1.373 (5)
C8—C20	1.381 (4)	C14—C13	1.359 (5)
N2—C10	1.305 (4)	C2—H2	0.9300
C17—H17	0.9300	C2—C3	1.375 (5)
C17—C18	1.380 (4)	C3—H3	0.9300
C18—C21	1.475 (5)	C3—C4	1.351 (6)
C18—C19	1.395 (4)	C4—H4	0.9300
C7—H7A	0.9700	C13—H13	0.9300
C7—H7B	0.9700	C22—H22A	0.9700
C16—H16	0.9300	C22—H22B	0.9700
C16—C11	1.381 (4)	C22—C23	1.433 (7)
C16—C15	1.379 (5)	C23—H23A	0.9600
C21—O2	1.197 (4)	C23—H23B	0.9600
C11—C10	1.465 (4)	C23—H23C	0.9600

C21—O1—C22	117.9 (3)	N2—C10—N1	113.2 (3)
C8—N1—C7	124.3 (3)	N2—C10—C11	123.4 (3)
C10—N1—C8	106.5 (3)	C18—C19—H19	119.0
C10—N1—C7	129.2 (3)	C20—C19—C18	122.1 (3)
C5—C6—C7	117.8 (3)	C20—C19—H19	119.0
C1—C6—C7	123.1 (3)	C6—C1—H1	120.2
C1—C6—C5	119.1 (3)	C6—C1—C2	119.5 (3)
N2—C9—C8	109.8 (3)	C2—C1—H1	120.2
C17—C9—C8	119.5 (3)	C11—C12—H12	119.8
C17—C9—N2	130.7 (3)	C13—C12—C11	120.5 (4)
N1—C8—C9	105.6 (3)	C13—C12—H12	119.8
N1—C8—C20	131.8 (3)	C15—C14—H14	120.3
C20—C8—C9	122.6 (3)	C13—C14—H14	120.3
C10—N2—C9	104.9 (2)	C13—C14—C15	119.4 (4)
C9—C17—H17	120.8	C1—C2—H2	120.0
C9—C17—C18	118.4 (3)	C3—C2—C1	119.9 (4)
C18—C17—H17	120.8	C3—C2—H2	120.0
C17—C18—C21	117.9 (3)	C16—C15—Cl1	119.8 (3)
C17—C18—C19	120.6 (3)	C14—C15—Cl1	119.6 (3)
C19—C18—C21	121.5 (3)	C14—C15—C16	120.6 (4)
N1—C7—C6	114.5 (3)	C2—C3—H3	119.9
N1—C7—H7A	108.6	C4—C3—C2	120.2 (4)
N1—C7—H7B	108.6	C4—C3—H3	119.9
C6—C7—H7A	108.6	C5—C4—H4	120.0
C6—C7—H7B	108.6	C3—C4—C5	120.1 (4)
H7A—C7—H7B	107.6	C3—C4—H4	120.0
C11—C16—H16	120.1	C12—C13—H13	119.5
C15—C16—H16	120.1	C14—C13—C12	121.0 (4)
C15—C16—C11	119.8 (3)	C14—C13—H13	119.5
O1—C21—C18	112.3 (3)	O1—C22—H22A	110.1
O2—C21—O1	122.8 (3)	O1—C22—H22B	110.1
O2—C21—C18	124.9 (4)	H22A—C22—H22B	108.4
C16—C11—C10	121.8 (3)	C23—C22—O1	108.0 (4)

C16—C11—C12	118.8 (3)	C23—C22—H22A	110.1
C12—C11—C10	119.4 (3)	C23—C22—H22B	110.1
C8—C20—H20	121.6	C22—C23—H23A	109.5
C19—C20—C8	116.9 (3)	C22—C23—H23B	109.5
C19—C20—H20	121.6	C22—C23—H23C	109.5
C6—C5—H5	119.4	H23A—C23—H23B	109.5
C4—C5—C6	121.2 (4)	H23A—C23—H23C	109.5
C4—C5—H5	119.4	H23B—C23—H23C	109.5
N1—C10—C11	123.4 (3)		

N1—C8—C20—C19	179.6 (3)	C16—C11—C10—N1	48.3 (5)
C6—C5—C4—C3	−0.3 (6)	C16—C11—C10—N2	−132.2 (3)
C6—C1—C2—C3	0.3 (5)	C16—C11—C12—C13	0.0 (5)
C9—C8—C20—C19	0.7 (5)	C21—O1—C22—C23	171.8 (5)
C9—N2—C10—N1	0.6 (4)	C21—C18—C19—C20	−179.2 (3)
C9—N2—C10—C11	−178.9 (3)	C11—C16—C15—Cl1	178.5 (2)
C9—C17—C18—C21	179.0 (3)	C11—C16—C15—C14	0.4 (5)
C9—C17—C18—C19	0.5 (5)	C11—C12—C13—C14	0.0 (6)
C8—N1—C7—C6	83.0 (4)	C5—C6—C7—N1	−177.5 (3)
C8—N1—C10—N2	−1.1 (4)	C5—C6—C1—C2	0.6 (5)
C8—N1—C10—C11	178.5 (3)	C10—N1—C8—C9	1.0 (3)
C8—C9—N2—C10	0.1 (3)	C10—N1—C8—C20	−178.0 (3)
C8—C9—C17—C18	0.3 (5)	C10—N1—C7—C6	−100.5 (4)
C8—C20—C19—C18	0.2 (5)	C10—C11—C12—C13	−178.9 (3)
N2—C9—C8—N1	−0.7 (3)	C19—C18—C21—O1	−6.7 (5)
N2—C9—C8—C20	178.4 (3)	C19—C18—C21—O2	173.0 (4)
N2—C9—C17—C18	−178.9 (3)	C1—C6—C7—N1	2.5 (4)
C17—C9—C8—N1	179.9 (3)	C1—C6—C5—C4	−0.6 (5)
C17—C9—C8—C20	−0.9 (5)	C1—C2—C3—C4	−1.2 (6)
C17—C9—N2—C10	179.4 (3)	C12—C11—C10—N1	−132.8 (3)
C17—C18—C21—O1	174.8 (3)	C12—C11—C10—N2	46.6 (5)
C17—C18—C21—O2	−5.5 (5)	C2—C3—C4—C5	1.2 (7)
C17—C18—C19—C20	−0.7 (5)	C15—C16—C11—C10	178.6 (3)
C7—N1—C8—C9	178.2 (3)	C15—C16—C11—C12	−0.3 (5)
C7—N1—C8—C20	−0.9 (5)	C15—C14—C13—C12	0.2 (6)
C7—N1—C10—N2	−178.0 (3)	C13—C14—C15—Cl1	−178.4 (3)
C7—N1—C10—C11	1.5 (5)	C13—C14—C15—C16	−0.4 (6)
C7—C6—C5—C4	179.4 (3)	C22—O1—C21—C18	−179.5 (3)
C7—C6—C1—C2	−179.5 (3)	C22—O1—C21—O2	0.8 (6)

Hydrogen-bond geometry (Å, º)

*Cg*4 is the centroid of the C11–C16 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···O2^{i}	0.93	2.54	3.358 (4)	148
C20—H20···*Cg*4^{ii}	0.93	2.87	3.757 (4)	159

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