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ISSN 2414-3146

1-Benzyl-5-chloroindoline-2,3-dione

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Received 25 May 2016
Accepted 26 May 2016

Edited by W. T. A. Harrison, University of Aberdeen, Scotland

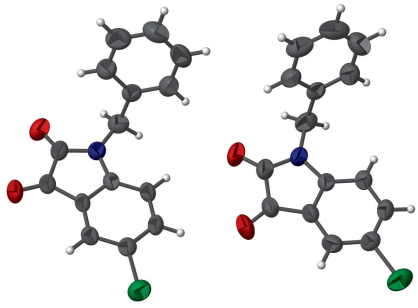
Keywords: crystal structure; indoline; hydrogen bonding; π–π stacking.

CCDC reference: 1482161

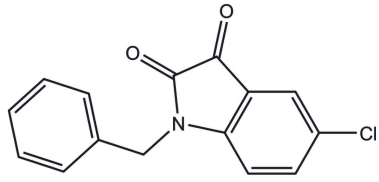
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{15}H_{10}ClNO_2$, crystallizes with two molecules (*A* and *B*) in the asymmetric unit, which have almost identical conformations (r.m.s. overlay fit = 0.057 Å). In molecule *A*, the dihedral angle between the indole ring system (r.m.s. deviation = 0.025 Å) and the phenyl group is 71.39 (8)°. Equivalent data for molecule *B* are 0.023 Å and 71.43 (9)°. In the crystal, the *A* and *B* molecules are linked by a C—H···O hydrogen bond and aromatic π–π stacking is also observed [shortest centroid–centroid separation = 3.5810 (11) Å].

3D view



Chemical scheme



Structure description

5-Chloro-indoline-2,3-dione has been used as a starting material for a variety of chemical reactions such as 1,3-dipolar cycloaddition (Ranjith Kumar *et al.*, 2009) and in the synthesis of several heterocyclic systems (Kharbach *et al.*, 2016). As part of our studies in this area, the synthesis and structure of the title compound, $C_{15}H_{10}ClNO_2$, are now described.

The title compound crystallizes with two molecules (*A* and *B*) in the asymmetric unit (Fig. 1). In each molecule, the indoline ring system is almost planar, with the largest deviation from the mean plane being 0.0230 (17) Å in molecule *A* and 0.0418 (18) Å in molecule *B*. The conformation of the two molecules are almost identical, as indicated by the angles of inclination of the indole moiety with respect to the benzyl ring system, the dihedral angles being 71.43 (9) and 71.39 (8)° in molecules *A* and *B*, respectively.

In the crystal, the *A* and *B* molecules are linked by a C—H···O hydrogen bond (Table 1) and aromatic π–π stacking is also observed [shortest centroid–centroid separation = 3.5810 (11) Å].

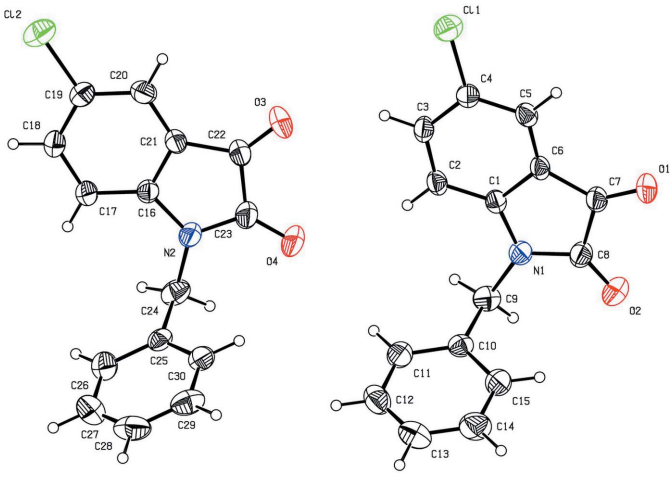


Figure 1
The molecular structure of the title molecule, showing displacement ellipsoids drawn at the 30% probability level.

Synthesis and crystallization

To a solution of 5-chloro-1*H*-indole-2,3-dione (0.4 g, 2,20 mmol) in *N*,*N*-dimethylformamide (25 ml), were added (0.5 g, 3,3 mmol) K_2CO_3, tetra-*n*-butylammonium fluoride (0.1 g, 0.3 mmol), and benzyl chloride (0.27 ml, 2,42 mmol)·The reaction mixture was stirred for 48 h at room temperature. After filtration the solution was evaporated under reduced pressure. The residue obtained was recrystallized from ethanol solution to afford the title compound as red crystals in a yield of 72% (m.p. 413 K)

Refinement

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

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O3	0.93	2.32	3.198 (3)	157

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_{10}ClNO_2$
M_r	271.69
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	296
a, b, c (Å)	4.4576 (2), 27.6646 (11), 20.9530 (8)
β (°)	93.870 (2)
V (Å^3)	2577.98 (18)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.29
Crystal size (mm)	0.32 × 0.26 × 0.19
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)
T_{min}, T_{max}	0.694, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	44717, 6252, 4206
R_{int}	0.034
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.667
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.043, 0.118, 1.02
No. of reflections	6252
No. of parameters	343
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.22, −0.29

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

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full crystallographic data

IUCrData (2016). **1**, x160854 [doi:10.1107/S2414314616008543]

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Crystal data

$C_{15}H_{10}ClNO_2$
M_r = 271.69
Monoclinic, $P2_1/n$
a = 4.4576 (2) Å
b = 27.6646 (11) Å
c = 20.9530 (8) Å
β = 93.870 (2)°
V = 2577.98 (18) Å^3
Z = 8
$F(000)$ = 1120
D_x = 1.400 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9947 reflections
θ = 2.4–25.1°
μ = 0.29 mm^{-1}
T = 296 K
Block, red
0.32 × 0.26 × 0.19 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2009)
T_{min} = 0.694, T_{max} = 0.746
44717 measured reflections
6252 independent reflections
4206 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 28.3°, θ_{min} = 2.4°
h = −5→5
k = −36→36
l = −27→27

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.118
S = 1.02
6252 reflections
343 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0466P)^2 + 0.6966P]$ 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

Experimental. SADABS-2014/5 (Bruker,2014/5) was used for absorption correction. wR2(int) was 0.0610 before and 0.0474 after correction. The Ratio of minimum to maximum transmission is 0.9304. The $\lambda/2$ correction factor is Not present.

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	0.89958 (12)	0.43330 (2)	0.48461 (2)	0.06747 (16)
Cl2	1.48632 (14)	0.11968 (2)	0.42404 (3)	0.08210 (19)
N1	0.0180 (3)	0.46593 (5)	0.26720 (7)	0.0491 (3)
O1	0.1339 (4)	0.57466 (5)	0.34834 (7)	0.0820 (5)
O2	−0.2505 (4)	0.53491 (6)	0.24114 (7)	0.0808 (4)
N2	0.6629 (4)	0.22139 (6)	0.23884 (7)	0.0589 (4)
C1	0.2383 (4)	0.45266 (5)	0.31566 (8)	0.0418 (4)
C6	0.3177 (4)	0.49196 (5)	0.35516 (8)	0.0436 (4)
C16	0.8647 (4)	0.19261 (6)	0.27710 (8)	0.0464 (4)
C10	0.0785 (4)	0.43138 (6)	0.16009 (8)	0.0480 (4)
C25	0.7006 (4)	0.21277 (6)	0.12230 (8)	0.0489 (4)
C5	0.5237 (4)	0.48727 (6)	0.40690 (8)	0.0468 (4)
H5	0.5764	0.5135	0.4330	0.056*
C4	0.6490 (4)	0.44222 (6)	0.41863 (8)	0.0465 (4)
C3	0.5724 (4)	0.40332 (6)	0.37927 (8)	0.0505 (4)
H3	0.6612	0.3734	0.3881	0.061*
C2	0.3667 (4)	0.40793 (6)	0.32713 (8)	0.0486 (4)
H2	0.3168	0.3817	0.3007	0.058*
O4	0.4619 (6)	0.29741 (7)	0.24693 (8)	0.1259 (8)
C21	0.9722 (5)	0.21743 (6)	0.33183 (8)	0.0556 (5)
C20	1.1657 (5)	0.19600 (7)	0.37758 (9)	0.0599 (5)
H20	1.2362	0.2126	0.4141	0.072*
C17	0.9515 (4)	0.14584 (6)	0.26680 (9)	0.0520 (4)
H17	0.8824	0.1291	0.2303	0.062*
C11	0.2055 (4)	0.38866 (7)	0.14143 (10)	0.0600 (5)
H11	0.1789	0.3606	0.1648	0.072*
C9	−0.1098 (4)	0.43402 (7)	0.21675 (9)	0.0561 (5)
H9A	−0.3091	0.4455	0.2027	0.067*
H9B	−0.1308	0.4018	0.2342	0.067*
C19	1.2502 (4)	0.14898 (7)	0.36694 (8)	0.0534 (4)
C7	0.1390 (5)	0.53319 (6)	0.33089 (9)	0.0551 (4)
C30	0.7950 (5)	0.25819 (7)	0.10518 (9)	0.0608 (5)
H30	0.7444	0.2849	0.1291	0.073*
C8	−0.0624 (4)	0.51317 (7)	0.27356 (9)	0.0567 (5)
C18	1.1458 (4)	0.12459 (6)	0.31285 (9)	0.0565 (5)
H18	1.2075	0.0929	0.3070	0.068*
C15	0.1231 (5)	0.47248 (7)	0.12408 (9)	0.0637 (5)
H15	0.0395	0.5017	0.1357	0.076*
O3	0.8623 (7)	0.29835 (6)	0.36596 (9)	0.1378 (10)
C12	0.3732 (5)	0.38726 (9)	0.08782 (11)	0.0717 (6)

H12	0.4579	0.3583	0.0756	0.086*
C24	0.5105 (4)	0.20621 (8)	0.17810 (9)	0.0644 (5)
H24A	0.3268	0.2248	0.1706	0.077*
H24B	0.4553	0.1724	0.1811	0.077*
C26	0.7800 (5)	0.17377 (8)	0.08660 (11)	0.0725 (6)
H26	0.7196	0.1429	0.0976	0.087*
C29	0.9621 (5)	0.26426 (9)	0.05342 (10)	0.0757 (6)
H29	1.0230	0.2951	0.0421	0.091*
C13	0.4138 (5)	0.42790 (10)	0.05335 (11)	0.0769 (6)
H13	0.5260	0.4268	0.0175	0.092*
C23	0.6255 (6)	0.26494 (8)	0.26680 (10)	0.0837 (7)
C14	0.2892 (6)	0.47045 (9)	0.07147 (11)	0.0806 (7)
H14	0.3175	0.4983	0.0478	0.097*
C28	1.0399 (6)	0.22532 (12)	0.01830 (11)	0.0878 (8)
H28	1.1549	0.2294	−0.0167	0.105*
C22	0.8338 (7)	0.26512 (8)	0.32918 (10)	0.0838 (7)
C27	0.9474 (7)	0.18010 (11)	0.03494 (12)	0.0937 (8)
H27	0.9990	0.1535	0.0109	0.112*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0701 (3)	0.0689 (3)	0.0622 (3)	0.0014 (2)	−0.0044 (2)	0.0077 (2)
Cl2	0.0794 (4)	0.0920 (4)	0.0726 (3)	0.0125 (3)	−0.0121 (3)	0.0205 (3)
N1	0.0558 (9)	0.0433 (8)	0.0488 (8)	−0.0013 (6)	0.0066 (7)	0.0031 (6)
O1	0.1337 (14)	0.0374 (7)	0.0748 (10)	0.0197 (8)	0.0069 (9)	−0.0047 (6)
O2	0.0923 (11)	0.0728 (10)	0.0758 (10)	0.0292 (9)	−0.0041 (8)	0.0133 (8)
N2	0.0693 (10)	0.0558 (9)	0.0523 (9)	0.0217 (8)	0.0098 (8)	0.0083 (7)
C1	0.0463 (9)	0.0358 (8)	0.0447 (8)	−0.0021 (7)	0.0129 (7)	0.0010 (6)
C6	0.0553 (10)	0.0308 (8)	0.0465 (9)	0.0000 (7)	0.0166 (7)	0.0006 (6)
C16	0.0516 (10)	0.0430 (9)	0.0457 (9)	0.0047 (7)	0.0105 (7)	0.0037 (7)
C10	0.0464 (9)	0.0504 (10)	0.0459 (9)	−0.0078 (8)	−0.0066 (7)	−0.0006 (7)
C25	0.0444 (9)	0.0526 (10)	0.0481 (9)	0.0034 (7)	−0.0097 (7)	0.0061 (7)
C5	0.0578 (10)	0.0369 (8)	0.0468 (9)	−0.0062 (7)	0.0119 (8)	−0.0029 (7)
C4	0.0488 (9)	0.0451 (9)	0.0469 (9)	−0.0004 (7)	0.0118 (7)	0.0031 (7)
C3	0.0595 (11)	0.0357 (9)	0.0577 (10)	0.0078 (8)	0.0152 (8)	0.0035 (7)
C2	0.0618 (11)	0.0334 (8)	0.0518 (9)	−0.0009 (7)	0.0117 (8)	−0.0048 (7)
O4	0.197 (2)	0.0971 (13)	0.0846 (12)	0.0978 (15)	0.0187 (13)	0.0159 (10)
C21	0.0792 (13)	0.0421 (9)	0.0467 (9)	0.0079 (9)	0.0128 (9)	−0.0020 (7)
C20	0.0810 (14)	0.0544 (11)	0.0443 (9)	−0.0040 (10)	0.0030 (9)	−0.0040 (8)
C17	0.0619 (11)	0.0399 (9)	0.0538 (10)	0.0006 (8)	0.0006 (8)	−0.0041 (7)
C11	0.0643 (12)	0.0506 (11)	0.0629 (12)	−0.0039 (9)	−0.0119 (10)	−0.0024 (9)
C9	0.0557 (11)	0.0571 (11)	0.0549 (10)	−0.0132 (9)	0.0003 (8)	0.0017 (8)
C19	0.0537 (10)	0.0527 (11)	0.0538 (10)	0.0008 (8)	0.0036 (8)	0.0092 (8)
C7	0.0757 (12)	0.0393 (9)	0.0521 (10)	0.0073 (9)	0.0182 (9)	0.0036 (8)
C30	0.0744 (13)	0.0535 (11)	0.0532 (11)	0.0010 (9)	−0.0055 (10)	0.0050 (8)
C8	0.0664 (12)	0.0484 (10)	0.0567 (10)	0.0107 (9)	0.0136 (9)	0.0080 (8)
C18	0.0651 (12)	0.0414 (9)	0.0628 (11)	0.0081 (8)	0.0020 (9)	−0.0004 (8)

C15	0.0784 (14)	0.0528 (11)	0.0606 (12)	−0.0021 (10)	0.0098 (10)	0.0044 (9)
O3	0.262 (3)	0.0681 (11)	0.0817 (12)	0.0613 (14)	0.0030 (15)	−0.0282 (9)
C12	0.0679 (13)	0.0734 (15)	0.0726 (14)	0.0055 (11)	−0.0049 (11)	−0.0232 (12)
C24	0.0523 (11)	0.0772 (14)	0.0630 (12)	0.0059 (10)	−0.0022 (9)	0.0143 (10)
C26	0.0907 (16)	0.0543 (12)	0.0715 (14)	0.0025 (11)	−0.0026 (12)	−0.0034 (10)
C29	0.0802 (15)	0.0833 (16)	0.0622 (13)	−0.0167 (12)	−0.0043 (11)	0.0214 (12)
C13	0.0771 (15)	0.0949 (18)	0.0600 (12)	−0.0107 (13)	0.0141 (11)	−0.0138 (12)
C23	0.125 (2)	0.0678 (14)	0.0607 (12)	0.0473 (14)	0.0264 (13)	0.0102 (11)
C14	0.1027 (18)	0.0774 (16)	0.0638 (13)	−0.0130 (13)	0.0205 (13)	0.0109 (11)
C28	0.0759 (16)	0.137 (3)	0.0511 (12)	0.0076 (16)	0.0073 (11)	0.0098 (14)
C22	0.144 (2)	0.0541 (12)	0.0549 (12)	0.0337 (13)	0.0206 (13)	−0.0019 (10)
C27	0.117 (2)	0.0932 (19)	0.0712 (16)	0.0253 (17)	0.0095 (15)	−0.0180 (14)

Geometric parameters (Å, º)

Cl1—C4	1.7355 (18)	C20—H20	0.9300
Cl2—C19	1.7399 (18)	C20—C19	1.376 (3)
N1—C1	1.413 (2)	C17—H17	0.9300
N1—C9	1.463 (2)	C17—C18	1.384 (2)
N1—C8	1.364 (2)	C11—H11	0.9300
O1—C7	1.205 (2)	C11—C12	1.391 (3)
O2—C8	1.204 (2)	C9—H9A	0.9700
N2—C16	1.410 (2)	C9—H9B	0.9700
N2—C24	1.463 (2)	C19—C18	1.373 (3)
N2—C23	1.355 (3)	C7—C8	1.553 (3)
C1—C6	1.397 (2)	C30—H30	0.9300
C1—C2	1.377 (2)	C30—C29	1.367 (3)
C6—C5	1.379 (2)	C18—H18	0.9300
C6—C7	1.463 (2)	C15—H15	0.9300
C16—C21	1.394 (2)	C15—C14	1.370 (3)
C16—C17	1.372 (2)	O3—C22	1.201 (3)
C10—C11	1.378 (3)	C12—H12	0.9300
C10—C9	1.501 (3)	C12—C13	1.355 (3)
C10—C15	1.386 (2)	C24—H24A	0.9700
C25—C30	1.380 (3)	C24—H24B	0.9700
C25—C24	1.501 (3)	C26—H26	0.9300
C25—C26	1.373 (3)	C26—C27	1.367 (3)
C5—H5	0.9300	C29—H29	0.9300
C5—C4	1.381 (2)	C29—C28	1.362 (4)
C4—C3	1.385 (2)	C13—H13	0.9300
C3—H3	0.9300	C13—C14	1.366 (3)
C3—C2	1.384 (3)	C23—C22	1.551 (4)
C2—H2	0.9300	C14—H14	0.9300
O4—C23	1.213 (3)	C28—H28	0.9300
C21—C20	1.379 (3)	C28—C27	1.370 (4)
C21—C22	1.456 (3)	C27—H27	0.9300
C1—N1—C9	125.50 (14)	C20—C19—Cl2	119.23 (14)

C8—N1—C1	110.68 (14)	C18—C19—Cl2	119.61 (14)
C8—N1—C9	123.82 (16)	C18—C19—C20	121.14 (17)
C16—N2—C24	124.99 (15)	O1—C7—C6	131.16 (19)
C23—N2—C16	110.41 (16)	O1—C7—C8	123.55 (17)
C23—N2—C24	124.59 (17)	C6—C7—C8	105.29 (14)
C6—C1—N1	111.08 (14)	C25—C30—H30	119.7
C2—C1—N1	128.26 (15)	C29—C30—C25	120.7 (2)
C2—C1—C6	120.66 (16)	C29—C30—H30	119.7
C1—C6—C7	106.90 (15)	N1—C8—C7	105.98 (15)
C5—C6—C1	121.40 (15)	O2—C8—N1	126.95 (19)
C5—C6—C7	131.67 (15)	O2—C8—C7	127.06 (17)
C21—C16—N2	111.13 (15)	C17—C18—H18	119.1
C17—C16—N2	128.25 (16)	C19—C18—C17	121.86 (17)
C17—C16—C21	120.60 (16)	C19—C18—H18	119.1
C11—C10—C9	121.88 (17)	C10—C15—H15	119.7
C11—C10—C15	118.18 (18)	C14—C15—C10	120.6 (2)
C15—C10—C9	119.93 (17)	C14—C15—H15	119.7
C30—C25—C24	120.71 (18)	C11—C12—H12	119.8
C26—C25—C30	118.66 (19)	C13—C12—C11	120.4 (2)
C26—C25—C24	120.63 (18)	C13—C12—H12	119.8
C6—C5—H5	121.1	N2—C24—C25	112.91 (16)
C6—C5—C4	117.70 (15)	N2—C24—H24A	109.0
C4—C5—H5	121.1	N2—C24—H24B	109.0
C5—C4—Cl1	120.08 (13)	C25—C24—H24A	109.0
C5—C4—C3	121.00 (16)	C25—C24—H24B	109.0
C3—C4—Cl1	118.91 (13)	H24A—C24—H24B	107.8
C4—C3—H3	119.3	C25—C26—H26	119.8
C2—C3—C4	121.47 (16)	C27—C26—C25	120.4 (2)
C2—C3—H3	119.3	C27—C26—H26	119.8
C1—C2—C3	117.76 (15)	C30—C29—H29	119.9
C1—C2—H2	121.1	C28—C29—C30	120.2 (2)
C3—C2—H2	121.1	C28—C29—H29	119.9
C16—C21—C22	107.07 (17)	C12—C13—H13	120.2
C20—C21—C16	121.61 (16)	C12—C13—C14	119.7 (2)
C20—C21—C22	131.28 (18)	C14—C13—H13	120.2
C21—C20—H20	121.3	N2—C23—C22	106.44 (17)
C19—C20—C21	117.31 (17)	O4—C23—N2	126.8 (2)
C19—C20—H20	121.3	O4—C23—C22	126.8 (2)
C16—C17—H17	121.3	C15—C14—H14	119.6
C16—C17—C18	117.47 (16)	C13—C14—C15	120.7 (2)
C18—C17—H17	121.3	C13—C14—H14	119.6
C10—C11—H11	119.8	C29—C28—H28	120.2
C10—C11—C12	120.40 (19)	C29—C28—C27	119.5 (2)
C12—C11—H11	119.8	C27—C28—H28	120.2
N1—C9—C10	112.91 (14)	C21—C22—C23	104.91 (17)
N1—C9—H9A	109.0	O3—C22—C21	130.0 (2)
N1—C9—H9B	109.0	O3—C22—C23	125.1 (2)
C10—C9—H9A	109.0	C26—C27—C28	120.5 (2)

C10—C9—H9B	109.0	C26—C27—H27	119.7
H9A—C9—H9B	107.8	C28—C27—H27	119.7

Cl1—C4—C3—C2	177.96 (13)	O4—C23—C22—O3	−1.0 (5)
Cl2—C19—C18—C17	178.32 (15)	C21—C16—C17—C18	0.6 (3)
N1—C1—C6—C5	178.31 (14)	C21—C20—C19—Cl2	−178.39 (15)
N1—C1—C6—C7	−0.09 (18)	C21—C20—C19—C18	0.1 (3)
N1—C1—C2—C3	−177.86 (15)	C20—C21—C22—O3	2.5 (5)
O1—C7—C8—N1	177.33 (18)	C20—C21—C22—C23	−176.5 (2)
O1—C7—C8—O2	−2.4 (3)	C20—C19—C18—C17	−0.2 (3)
N2—C16—C21—C20	177.89 (17)	C17—C16—C21—C20	−0.7 (3)
N2—C16—C21—C22	−0.1 (2)	C17—C16—C21—C22	−178.68 (18)
N2—C16—C17—C18	−177.71 (17)	C11—C10—C9—N1	118.18 (18)
N2—C23—C22—C21	−2.0 (3)	C11—C10—C15—C14	0.0 (3)
N2—C23—C22—O3	178.9 (3)	C11—C12—C13—C14	0.0 (3)
C1—N1—C9—C10	−84.7 (2)	C9—N1—C1—C6	178.35 (15)
C1—N1—C8—O2	−177.55 (19)	C9—N1—C1—C2	−2.9 (3)
C1—N1—C8—C7	2.67 (18)	C9—N1—C8—O2	2.4 (3)
C1—C6—C5—C4	−0.2 (2)	C9—N1—C8—C7	−177.42 (15)
C1—C6—C7—O1	−178.3 (2)	C9—C10—C11—C12	178.53 (16)
C1—C6—C7—C8	1.63 (18)	C9—C10—C15—C14	−178.65 (19)
C6—C1—C2—C3	0.8 (2)	C7—C6—C5—C4	177.75 (17)
C6—C5—C4—Cl1	−177.70 (12)	C30—C25—C24—N2	−62.5 (2)
C6—C5—C4—C3	0.7 (2)	C30—C25—C26—C27	−0.4 (3)
C6—C7—C8—N1	−2.65 (19)	C30—C29—C28—C27	0.5 (4)
C6—C7—C8—O2	177.57 (19)	C8—N1—C1—C6	−1.75 (19)
C16—N2—C24—C25	−83.6 (2)	C8—N1—C1—C2	177.04 (17)
C16—N2—C23—O4	−178.2 (3)	C8—N1—C9—C10	95.4 (2)
C16—N2—C23—C22	1.9 (2)	C15—C10—C11—C12	0.0 (3)
C16—C21—C20—C19	0.3 (3)	C15—C10—C9—N1	−63.3 (2)
C16—C21—C22—O3	−179.7 (3)	C12—C13—C14—C15	−0.1 (4)
C16—C21—C22—C23	1.2 (2)	C24—N2—C16—C21	179.86 (17)
C16—C17—C18—C19	−0.2 (3)	C24—N2—C16—C17	−1.7 (3)
C10—C11—C12—C13	0.1 (3)	C24—N2—C23—O4	0.7 (4)
C10—C15—C14—C13	0.1 (3)	C24—N2—C23—C22	−179.14 (19)
C25—C30—C29—C28	−0.6 (3)	C24—C25—C30—C29	−178.42 (17)
C25—C26—C27—C28	0.4 (4)	C24—C25—C26—C27	178.5 (2)
C5—C6—C7—O1	3.5 (3)	C26—C25—C30—C29	0.5 (3)
C5—C6—C7—C8	−176.54 (17)	C26—C25—C24—N2	118.6 (2)
C5—C4—C3—C2	−0.5 (3)	C29—C28—C27—C26	−0.4 (4)
C4—C3—C2—C1	−0.3 (3)	C23—N2—C16—C21	−1.2 (2)
C2—C1—C6—C5	−0.6 (2)	C23—N2—C16—C17	177.2 (2)
C2—C1—C6—C7	−178.99 (15)	C23—N2—C24—C25	97.6 (2)
O4—C23—C22—C21	178.2 (3)	C22—C21—C20—C19	177.8 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O3	0.93	2.32	3.198 (3)	157