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ISSN 2414-3146

1-(3-Chloro-6-nitro-1*H*-indazol-1-yl)ethan-1-one

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Received 19 June 2017
Accepted 19 August 2017

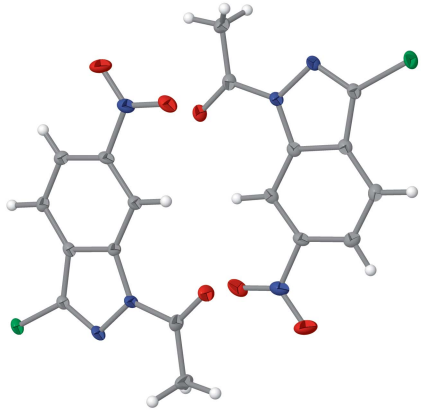
Edited by P. Bombicz, Hungarian Academy of Sciences, Hungary

Keywords: crystal structure; indazole; π–π stacking.

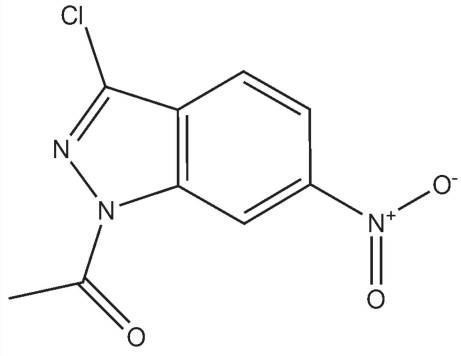
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title compound, $C_9H_6ClN_3O_3$, contains one full molecule in a general position and a half molcule sitting on a crystallographic mirror plane. In the crystal, molecules form stacks extending along the *b*-axis direction through a combination of offset π–π stacking between indazole units and C—Cl$\cdots\pi$(ring) interactions with the six-membered rings of the same units. Elaboration of the C—Cl$\cdots\pi$(ring) interactions along the *a*-axis direction forms slabs of molecules parallel to [001]. The stacks are joined by a combination of C—H$\cdots$O and C—H$\cdots$N hydrogen bonds.

3D view



Chemical scheme



Structure description

Studies of the structure and physicochemical properties of the indazole ring have been reviewed (Abbassi *et al.*, 2014; Li *et al.*, 2003; Lee *et al.*, 2001). Indazole is a frequently found motif in drug substances with important biological activities, such as antimicrobial (Patel *et al.*, 1999) and anti-inflammatory activities (Lin *et al.*, 2008), and anticancer effects (Zhu *et al.*, 2007). As a continuation of our studies of indazole derivatives (Mohamed Abdelahi *et al.*, 2017*a*,*b*,*c*), we report the synthesis and structure of the title compound (Fig. 1).

The asymmetric unit of the title compound consists of one molecule in a general position and a half molecule located on a crystallographic mirror plane at y = 1/4. The indazole portion of the former is planar to within 0.007 (1) Å (C16) and the dihedral angle between its mean plane and the mirror on which the latter lies is 4.82 (3) Å. For the overlay of the two independent molecules, values of 0.0130 and 0.0288 Å are obtained, respectively, for the r.m.s. deviation and the maximum deviation. In the crystal, molecules form stacks extending along the *b*-axis direction. One element of the stack is a dimer formed by pairwise head-to-tail offset π–π stacking interactions between the indazole

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···O1^{i}	0.89 (2)	2.46 (2)	3.212 (3)	142 (2)
C9—H9B···N2^{ii}	0.92 (3)	2.65 (3)	3.554 (3)	166 (2)
C13—H13···O4^{ii}	0.91 (2)	2.520 (19)	3.235 (2)	135.4 (15)
C18—H18A···N5^{i}	0.95 (2)	2.62 (2)	3.530 (2)	159.9 (16)

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

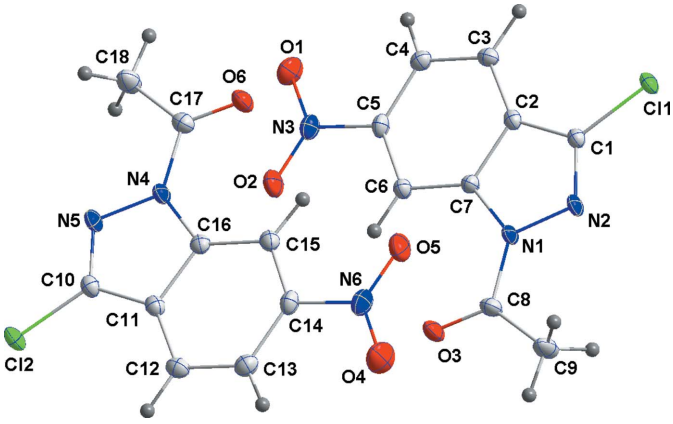


Figure 1
The asymmetric unit of the title compound, with the atom-labelling scheme and 50% probability ellipsoids.

portions of two molecules sitting on general positions [Fig. 2; $Cg4\cdots Cg5^{iii}$ = 3.6023 (8) Å]. The dimers are connected across the crystallographic mirror plane by complementary C10—Cl2···π($Cg2$) and C1—Cl1···π($Cg5$) interactions with the molecule sitting on the mirror [Fig. 2; Cl1···$Cg5^{i}$ = 3.2306 (6) Å, C1···$Cg5^{i}$ = 3.748 (1) Å and C1—Cl1···$Cg5^{i}$ = 95.13 (5)°; Cl2^{i}···$Cg2$ = 3.4284 (6) Å, C10^{i}···$Cg2$ = 3.4284 (4) Å and C10^{i}—Cl2^{i}···$Cg2$ = 91.73 (5)°]. Elaboration of the C10—Cl2···π($Cg2$) and C1—Cl1···π($Cg5$) interactions

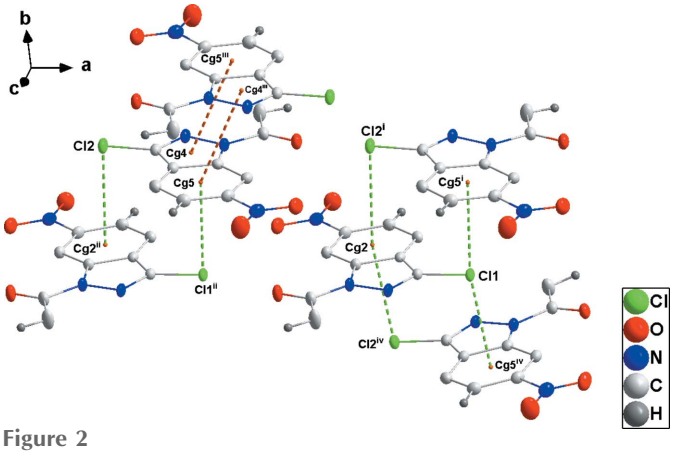


Figure 2
Detail of the π–π stacking (orange dashed lines) and C—Cl···π(ring) (green dashed lines) interactions [symmetry codes: (i) $x+1, y, z$; (ii) $x-1, y, z$; (iii) $-x+1, -y+1, -z+1$; (iv) $x+1, -y+\frac{1}{2}, z$.] $Cg2$ = centroid(C2–C7 ring); $Cg4$ = centroid (C10/C11/C16/N4/N5 ring); $Cg5$ = centroid(C11–C16 ring).

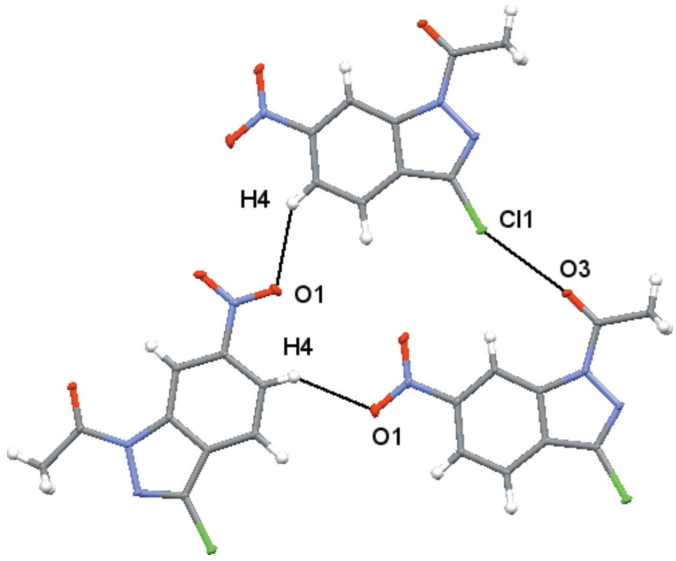


Figure 3
Detail of the $R_3^3(19)$ graph set formed by the Cl1···O3 interaction and two C4—H4···O1 hydrogen bonds. Genreic atom labels without symmetry codes have been used.

along the a-axis direction forms slabs of molecules parallel to [001]. The stacks are joined by a combination of C—H···O and C—H···N hydrogen bonds, as well as short Cl···O contacts of 2.964 (2) and 2.982 (1) Å with the nitro groups of neighbouring molecules (Table 1 and Fig. 4). As shown in Fig. 3, an $R_3^3(19)$ graph set is formed by two C—H···O hydrogen bonds and one Cl···O interaction for the molecule in the general position. A corresponding set is formed with the molecule in the special position.

Synthesis and crystallization

A mixture of 3-chloro-6-nitro-1H-indazole (0.6 g, 3 mmol), acetic acid (2 ml) and acetic anhydride (10 ml) was heated

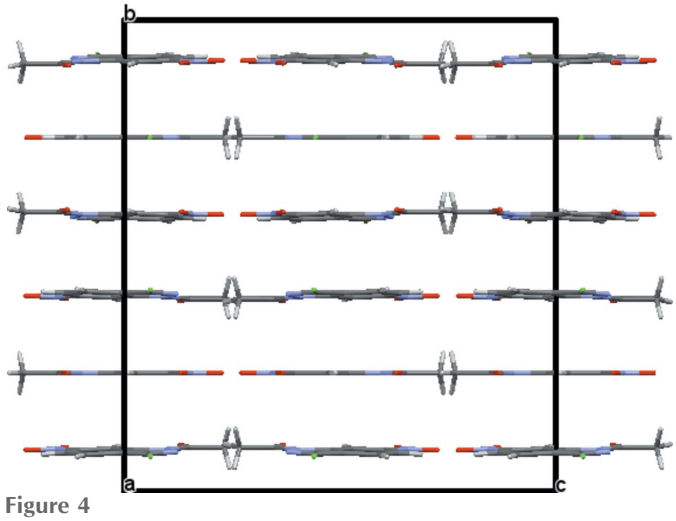


Figure 4
Packing viewed along the a-axis direction, showing the layer structure. The π-stacking and C—Cl···π(ring) interactions (omitted for clarity) run along the b-axis direction.

under reflux for 24 h. After completion of the reaction (monitored by thin-layer chromatography), the solvent was removed under vacuum. The residue obtained was recrystallized from ethanol to afford the title compound as colourless crystals (yield 75%).

Refinement

Crystal and refinement details are presented in Table 2.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_9H_6ClN_3O_3$
M_r	239.62
Crystal system, space group	Orthorhombic, *Pnma*
Temperature (K)	100
a, b, c (Å)	8.5638 (5), 19.2608 (12), 17.6509 (10)
V (Å^3)	2911.4 (3)
Z	12
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.39
Crystal size (mm)	0.22 × 0.21 × 0.06
Data collection	
Diffractometer	Bruker SMART APEX CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.78, 0.98
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	53113, 3866, 3016
R_{int}	0.061
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.676
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.040, 0.110, 1.06
No. of reflections	3866
No. of parameters	281
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.76, −0.30

Computer programs: *APEX3* (Bruker, 2016), *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Bruker, 2016).

Acknowledgements

JTM thanks Tulane University for support of the Tulane Crystallography Laboratory.

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full crystallographic data

IUCrData (2017). **2**, x171202 [https://doi.org/10.1107/S2414314617012020]

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Crystal data

$C_9H_6ClN_3O_3$
M_r = 239.62
Orthorhombic, *Pnma*
a = 8.5638 (5) Å
b = 19.2608 (12) Å
c = 17.6509 (10) Å
V = 2911.4 (3) Å^3
Z = 12
F(000) = 1464
D_x = 1.640 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 9981 reflections
θ = 2.6–28.2°
μ = 0.39 mm^{-1}
T = 100 K
Plate, colourless
0.22 × 0.21 × 0.06 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.3333 pixels mm^{-1}
φ and *ω* scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
T_{min} = 0.78, T_{max} = 0.98
53113 measured reflections
3866 independent reflections
3016 reflections with $I > 2\sigma(I)$
R_{int} = 0.061
θ_{max} = 28.7°, θ_{min} = 1.6°
h = −11→11
k = −25→25
l = −23→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.110
S = 1.06
3866 reflections
281 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0599P)^2 + 0.705P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.76 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Special details

Experimental. The diffraction data were obtained from 3 sets of 400 frames, each of width 0.5° in *ω*, colllected at *φ* = 0.00, 90.00 and 180.00° and 2 sets of 800 frames, each of width 0.45° in *φ*, collected at *ω* = –30.00 and 210.00°. The scan time was 25 sec/frame.

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	1.41305 (5)	0.2500	0.55876 (3)	0.01626 (13)
O1	0.7647 (2)	0.2500	0.27364 (9)	0.0290 (4)
O2	0.60283 (18)	0.2500	0.36813 (9)	0.0231 (4)
O3	0.72598 (17)	0.2500	0.63055 (8)	0.0212 (3)
N1	0.97947 (19)	0.2500	0.59702 (10)	0.0145 (3)
N2	1.13404 (19)	0.2500	0.61869 (10)	0.0155 (3)
N3	0.7358 (2)	0.2500	0.34206 (10)	0.0185 (4)
C1	1.2143 (2)	0.2500	0.55576 (11)	0.0133 (4)
C2	1.1184 (2)	0.2500	0.48943 (11)	0.0129 (4)
C3	1.1466 (2)	0.2500	0.41136 (12)	0.0148 (4)
H3	1.257 (3)	0.2500	0.3913 (15)	0.024 (6)*
C4	1.0184 (2)	0.2500	0.36359 (12)	0.0156 (4)
H4	1.042 (3)	0.2500	0.3142 (14)	0.014 (6)*
C5	0.8683 (2)	0.2500	0.39485 (11)	0.0156 (4)
C6	0.8350 (2)	0.2500	0.47147 (11)	0.0143 (4)
H6	0.733 (3)	0.2500	0.4899 (12)	0.010 (5)*
C7	0.9653 (2)	0.2500	0.51857 (11)	0.0133 (4)
C8	0.8598 (2)	0.2500	0.65156 (12)	0.0180 (4)
C9	0.9129 (3)	0.2500	0.73218 (13)	0.0260 (5)
H9A	0.978 (3)	0.2910 (11)	0.7411 (13)	0.046 (6)*
H9B	0.827 (4)	0.2500	0.7640 (17)	0.037 (8)*
Cl2	0.02758 (4)	0.42726 (2)	0.43856 (2)	0.01905 (11)
O4	0.67364 (16)	0.41371 (7)	0.72589 (7)	0.0386 (3)
O5	0.83539 (14)	0.40821 (6)	0.63194 (7)	0.0277 (3)
O6	0.71422 (12)	0.40330 (6)	0.36968 (6)	0.0206 (2)
N4	0.46081 (14)	0.41264 (6)	0.40256 (7)	0.0152 (3)
N5	0.30658 (13)	0.41789 (6)	0.38006 (7)	0.0158 (3)
N6	0.70329 (16)	0.41177 (7)	0.65786 (8)	0.0223 (3)
C10	0.22560 (17)	0.42214 (7)	0.44273 (8)	0.0151 (3)
C11	0.32115 (16)	0.42031 (7)	0.50930 (8)	0.0145 (3)
C12	0.29228 (18)	0.42324 (7)	0.58742 (9)	0.0172 (3)
H12	0.188 (2)	0.4277 (9)	0.6083 (11)	0.025 (5)*
C13	0.41978 (18)	0.41991 (8)	0.63526 (9)	0.0187 (3)
H13	0.405 (2)	0.4224 (8)	0.6865 (12)	0.022 (5)*
C14	0.57019 (17)	0.41413 (7)	0.60457 (9)	0.0169 (3)
C15	0.60411 (17)	0.41083 (7)	0.52825 (9)	0.0157 (3)

H15	0.711 (2)	0.4055 (8)	0.5104 (9)	0.015 (4)*
C16	0.47364 (17)	0.41386 (7)	0.48071 (8)	0.0142 (3)
C17	0.58083 (17)	0.40742 (7)	0.34803 (9)	0.0171 (3)
C18	0.5292 (2)	0.40755 (10)	0.26742 (9)	0.0244 (4)
H18A	0.617 (2)	0.4013 (10)	0.2350 (13)	0.037 (6)*
H18B	0.478 (2)	0.4507 (11)	0.2553 (12)	0.034 (5)*
H18C	0.454 (2)	0.3699 (10)	0.2578 (13)	0.040 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0087 (2)	0.0177 (3)	0.0224 (3)	0.000	0.00009 (17)	0.000
O1	0.0306 (9)	0.0417 (10)	0.0146 (8)	0.000	−0.0063 (7)	0.000
O2	0.0149 (7)	0.0292 (9)	0.0252 (8)	0.000	−0.0065 (6)	0.000
O3	0.0110 (7)	0.0346 (9)	0.0181 (8)	0.000	0.0007 (6)	0.000
N1	0.0083 (7)	0.0222 (9)	0.0131 (8)	0.000	−0.0019 (6)	0.000
N2	0.0078 (7)	0.0200 (9)	0.0188 (8)	0.000	−0.0030 (6)	0.000
N3	0.0191 (9)	0.0190 (9)	0.0175 (9)	0.000	−0.0055 (7)	0.000
C1	0.0109 (8)	0.0132 (9)	0.0158 (9)	0.000	−0.0004 (7)	0.000
C2	0.0112 (9)	0.0102 (9)	0.0174 (10)	0.000	−0.0008 (7)	0.000
C3	0.0145 (9)	0.0142 (10)	0.0157 (9)	0.000	0.0030 (8)	0.000
C4	0.0178 (10)	0.0154 (10)	0.0135 (9)	0.000	0.0005 (8)	0.000
C5	0.0145 (9)	0.0170 (10)	0.0154 (10)	0.000	−0.0054 (8)	0.000
C6	0.0119 (9)	0.0163 (10)	0.0148 (9)	0.000	−0.0010 (7)	0.000
C7	0.0122 (9)	0.0153 (10)	0.0124 (9)	0.000	0.0002 (7)	0.000
C8	0.0138 (9)	0.0234 (11)	0.0168 (10)	0.000	0.0041 (8)	0.000
C9	0.0168 (10)	0.0482 (16)	0.0131 (10)	0.000	0.0025 (8)	0.000
Cl2	0.01007 (17)	0.0234 (2)	0.0237 (2)	0.00078 (13)	−0.00004 (13)	−0.00311 (13)
O4	0.0349 (7)	0.0635 (10)	0.0174 (6)	0.0032 (6)	−0.0067 (5)	−0.0010 (5)
O5	0.0171 (5)	0.0339 (7)	0.0320 (7)	−0.0015 (5)	−0.0070 (5)	0.0052 (5)
O6	0.0127 (5)	0.0268 (6)	0.0224 (6)	0.0012 (4)	0.0013 (4)	−0.0011 (4)
N4	0.0098 (5)	0.0199 (6)	0.0159 (6)	−0.0003 (4)	−0.0014 (5)	−0.0004 (5)
N5	0.0097 (6)	0.0196 (6)	0.0181 (6)	−0.0002 (4)	−0.0026 (5)	−0.0019 (5)
N6	0.0239 (7)	0.0239 (7)	0.0192 (7)	−0.0005 (5)	−0.0066 (5)	0.0019 (5)
C10	0.0123 (6)	0.0143 (7)	0.0185 (7)	−0.0003 (5)	−0.0008 (5)	−0.0010 (5)
C11	0.0128 (6)	0.0130 (7)	0.0176 (7)	−0.0011 (5)	−0.0006 (5)	−0.0004 (5)
C12	0.0167 (7)	0.0155 (7)	0.0194 (7)	−0.0005 (5)	0.0031 (6)	−0.0013 (5)
C13	0.0216 (8)	0.0185 (7)	0.0161 (7)	−0.0009 (6)	0.0000 (6)	−0.0004 (5)
C14	0.0170 (7)	0.0163 (7)	0.0172 (7)	−0.0005 (5)	−0.0053 (5)	0.0005 (5)
C15	0.0139 (7)	0.0142 (7)	0.0188 (7)	−0.0005 (5)	−0.0007 (6)	0.0016 (5)
C16	0.0142 (6)	0.0120 (7)	0.0165 (7)	−0.0013 (5)	−0.0003 (5)	0.0012 (5)
C17	0.0147 (7)	0.0174 (7)	0.0193 (7)	−0.0006 (5)	0.0027 (5)	−0.0005 (6)
C18	0.0185 (7)	0.0378 (10)	0.0168 (7)	0.0021 (7)	0.0013 (6)	−0.0036 (6)

Geometric parameters (Å, º)

Cl1—C1	1.703 (2)	O4—N6	1.2280 (18)
O1—N3	1.233 (2)	O5—N6	1.2222 (18)

O2—N3	1.228 (2)	O6—C17	1.2071 (18)
O3—C8	1.205 (3)	N4—N5	1.3829 (16)
N1—N2	1.378 (2)	N4—C16	1.3840 (19)
N1—C7	1.390 (3)	N4—C17	1.4116 (19)
N1—C8	1.406 (3)	N5—C10	1.3083 (18)
N2—C1	1.306 (3)	N6—C14	1.4785 (19)
N3—C5	1.468 (3)	C10—C11	1.432 (2)
C1—C2	1.430 (3)	C11—C12	1.402 (2)
C2—C3	1.399 (3)	C11—C16	1.406 (2)
C2—C7	1.408 (3)	C12—C13	1.382 (2)
C3—C4	1.384 (3)	C12—H12	0.97 (2)
C3—H3	1.01 (3)	C13—C14	1.402 (2)
C4—C5	1.399 (3)	C13—H13	0.91 (2)
C4—H4	0.89 (2)	C14—C15	1.380 (2)
C5—C6	1.382 (3)	C15—C16	1.399 (2)
C6—C7	1.391 (3)	C15—H15	0.975 (17)
C6—H6	0.93 (2)	C17—C18	1.490 (2)
C8—C9	1.494 (3)	C18—H18A	0.95 (2)
C9—H9A	0.98 (2)	C18—H18B	0.96 (2)
C9—H9B	0.92 (3)	C18—H18C	0.98 (2)
Cl2—C10	1.7003 (16)		

N2—N1—C7	111.11 (16)	C16—N4—C17	128.53 (12)
N2—N1—C8	120.67 (17)	C10—N5—N4	105.55 (12)
C7—N1—C8	128.22 (17)	O5—N6—O4	123.99 (14)
C1—N2—N1	105.63 (16)	O5—N6—C14	118.50 (13)
O2—N3—O1	123.61 (18)	O4—N6—C14	117.50 (14)
O2—N3—C5	118.60 (17)	N5—C10—C11	112.91 (13)
O1—N3—C5	117.79 (18)	N5—C10—Cl2	119.71 (11)
N2—C1—C2	113.19 (17)	C11—C10—Cl2	127.36 (11)
N2—C1—Cl1	119.97 (15)	C12—C11—C16	121.37 (13)
C2—C1—Cl1	126.84 (15)	C12—C11—C10	134.84 (14)
C3—C2—C7	121.37 (18)	C16—C11—C10	103.79 (13)
C3—C2—C1	134.99 (18)	C13—C12—C11	117.37 (14)
C7—C2—C1	103.63 (17)	C13—C12—H12	119.9 (11)
C4—C3—C2	117.59 (18)	C11—C12—H12	122.8 (11)
C4—C3—H3	122.0 (15)	C12—C13—C14	119.58 (14)
C2—C3—H3	120.4 (15)	C12—C13—H13	119.5 (12)
C3—C4—C5	119.23 (19)	C14—C13—H13	120.9 (12)
C3—C4—H4	114.7 (15)	C15—C14—C13	125.07 (14)
C5—C4—H4	126.1 (15)	C15—C14—N6	117.22 (13)
C6—C5—C4	125.13 (18)	C13—C14—N6	117.71 (13)
C6—C5—N3	117.49 (18)	C14—C15—C16	114.57 (13)
C4—C5—N3	117.38 (18)	C14—C15—H15	121.2 (10)
C5—C6—C7	114.79 (18)	C16—C15—H15	124.2 (10)
C5—C6—H6	122.4 (14)	N4—C16—C15	131.36 (14)
C7—C6—H6	122.8 (14)	N4—C16—C11	106.60 (12)
N1—C7—C6	131.68 (18)	C15—C16—C11	122.04 (14)

N1—C7—C2	106.43 (16)	O6—C17—N4	118.55 (14)
C6—C7—C2	121.89 (18)	O6—C17—C18	125.69 (14)
O3—C8—N1	118.86 (19)	N4—C17—C18	115.76 (13)
O3—C8—C9	125.63 (19)	C17—C18—H18A	109.8 (13)
N1—C8—C9	115.51 (18)	C17—C18—H18B	110.4 (13)
C8—C9—H9A	109.0 (14)	H18A—C18—H18B	109.6 (17)
C8—C9—H9B	109.8 (18)	C17—C18—H18C	110.9 (13)
H9A—C9—H9B	110.6 (17)	H18A—C18—H18C	108.6 (18)
N5—N4—C16	111.15 (12)	H18B—C18—H18C	107.5 (17)
N5—N4—C17	120.32 (12)		

C7—N1—N2—C1	0.000 (1)	C16—N4—N5—C10	−0.12 (15)
C8—N1—N2—C1	180.000 (1)	C17—N4—N5—C10	−179.72 (12)
N1—N2—C1—C2	0.000 (1)	N4—N5—C10—C11	0.31 (16)
N1—N2—C1—Cl1	180.000 (1)	N4—N5—C10—Cl2	−178.42 (10)
N2—C1—C2—C3	180.000 (1)	N5—C10—C11—C12	179.83 (15)
Cl1—C1—C2—C3	0.000 (1)	Cl2—C10—C11—C12	−1.6 (2)
N2—C1—C2—C7	0.000 (1)	N5—C10—C11—C16	−0.38 (16)
Cl1—C1—C2—C7	180.000 (1)	Cl2—C10—C11—C16	178.23 (11)
C7—C2—C3—C4	0.000 (1)	C16—C11—C12—C13	0.3 (2)
C1—C2—C3—C4	180.000 (1)	C10—C11—C12—C13	−179.91 (15)
C2—C3—C4—C5	0.000 (1)	C11—C12—C13—C14	0.3 (2)
C3—C4—C5—C6	0.000 (1)	C12—C13—C14—C15	−0.5 (2)
C3—C4—C5—N3	180.000 (1)	C12—C13—C14—N6	179.12 (13)
O2—N3—C5—C6	0.000 (1)	O5—N6—C14—C15	1.2 (2)
O1—N3—C5—C6	180.000 (1)	O4—N6—C14—C15	−179.00 (14)
O2—N3—C5—C4	180.000 (1)	O5—N6—C14—C13	−178.49 (13)
O1—N3—C5—C4	0.000 (1)	O4—N6—C14—C13	1.3 (2)
C4—C5—C6—C7	0.000 (1)	C13—C14—C15—C16	0.1 (2)
N3—C5—C6—C7	180.000 (1)	N6—C14—C15—C16	−179.49 (12)
N2—N1—C7—C6	180.000 (1)	N5—N4—C16—C15	−179.17 (14)
C8—N1—C7—C6	0.000 (1)	C17—N4—C16—C15	0.4 (2)
N2—N1—C7—C2	0.000 (1)	N5—N4—C16—C11	−0.11 (15)
C8—N1—C7—C2	180.000 (1)	C17—N4—C16—C11	179.44 (13)
C5—C6—C7—N1	180.000 (1)	C14—C15—C16—N4	179.41 (14)
C5—C6—C7—C2	0.000 (1)	C14—C15—C16—C11	0.5 (2)
C3—C2—C7—N1	180.000 (1)	C12—C11—C16—N4	−179.90 (12)
C1—C2—C7—N1	0.000 (1)	C10—C11—C16—N4	0.28 (14)
C3—C2—C7—C6	0.000 (1)	C12—C11—C16—C15	−0.7 (2)
C1—C2—C7—C6	180.000 (1)	C10—C11—C16—C15	179.45 (13)
N2—N1—C8—O3	180.000 (1)	N5—N4—C17—O6	179.59 (13)
C7—N1—C8—O3	0.000 (1)	C16—N4—C17—O6	0.1 (2)
N2—N1—C8—C9	0.000 (1)	N5—N4—C17—C18	−0.40 (19)
C7—N1—C8—C9	180.000 (1)	C16—N4—C17—C18	−179.92 (14)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···O1^{i}	0.89 (2)	2.46 (2)	3.212 (3)	142 (2)
C9—H9*B*···N2^{ii}	0.92 (3)	2.65 (3)	3.554 (3)	166 (2)
C13—H13···O4^{ii}	0.91 (2)	2.520 (19)	3.235 (2)	135.4 (15)
C18—H18*A*···N5^{i}	0.95 (2)	2.62 (2)	3.530 (2)	159.9 (16)

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