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(3*E*)-5-Chloro-3-(2-phenylhydrazinylidene)-1*H*-indol-2(3*H*)-one

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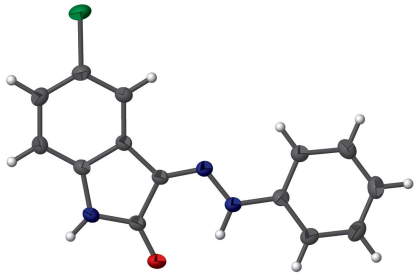
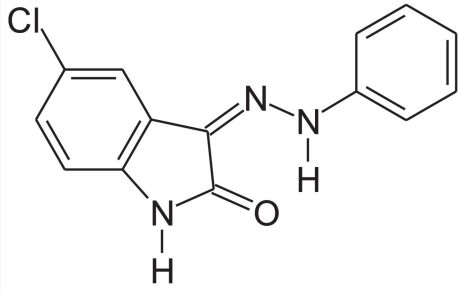
Structural data: full structural data are available from iucrdata.iucr.org

The reaction between 5-cholroisatin and phenylhydrazine yields the title compound, $C_{14}H_{10}ClN_3O$. The molecular structure deviates slightly from the ideal planarity, with an r.m.s. deviation of 0.1372 (12) Å for the non-H atoms. An N—H···O intramolecular interaction is observed, which supports an *E* conformation with respect to the C=N bond. In the crystal, molecules are linked by a pair of N—H···O interactions into an inversion dimer. The dimers are linked by weak C—H···Cl interactions, formng a tape structure along [101]. The tapes are also linked through a weak π–π interaction [centroid–centroid distance = 3.5773 (8) Å] into a layer parallel to ($\bar{1}$11). An *in silico* evaluation of the title compound with a topoisomerase enzyme was performed and the global free energy of −26.59 kJ mol^{-1} was found.

3D view



Chemical scheme



Structure description

The chemistry of isatin derivatives covers a wide range of scientific disciplines with special attention to medicinal chemistry (Vine *et al.*, 2013). As part of our ongoing research into isatin derivatives, we report herein the crystal structure of the title compound (common name: 5-chloroisatine-3-phenylhydrazone).

The title molecule is nearly planar, with the r.m.s. deviation for the non-H atoms being 0.1372 (12) Å for atom C11 (Fig. 1). In the crystal, molecules are linked by N—H···O and weak C—H···Cl interactions (Table 1) into a hydrogen-bonded tape structure along [101] (Fig. 2). In addition, a weak π–π interaction between the pyrrole and phenyl rings [centroid–centroid distance = 3.5773 (8) Å] connects the tapes, forming a layer parallel to

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H1*N3*···O1	0.95	2.00	2.7581 (12)	136
N1—H1*N1*···O1^{i}	0.89	1.97	2.8431 (12)	167
C14—H8···Cl1^{ii}	0.95	2.90	3.5476 (12)	127

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

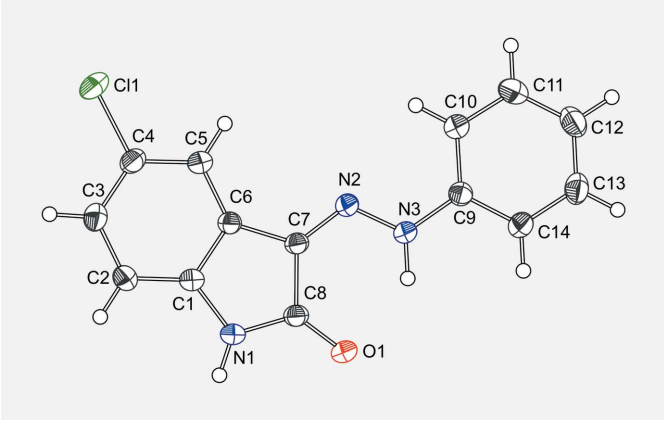


Figure 1
The molecular structure of the title compound, showing the atom labelling and displacement ellipsoids drawn at the 50% probability level.

($\bar{1}11$). C···C contacts of C2^{iii}···C9 = 3.2866 (15) Å, C7^{iii}···C7 = 3.3309 (14) Å and C13···C6^{iv} = 3.3888 (14) Å are also observed between adjacent tapes [Fig. 3; symmetry codes: (iii) $-x+1, -y+2, -z+1$; (iv) $-x+1, -y+1, -z+1$].

An *in silico* evaluation of the title compound with the DNA topoisomerase IIα was performed using *PatchDock* (Duhovny *et al.*, 2002; Schneidman-Duhovny *et al.*, 2005) and *FireDock* (Andrusier *et al.*, 2007; Mashiach *et al.*, 2008). The crystal data

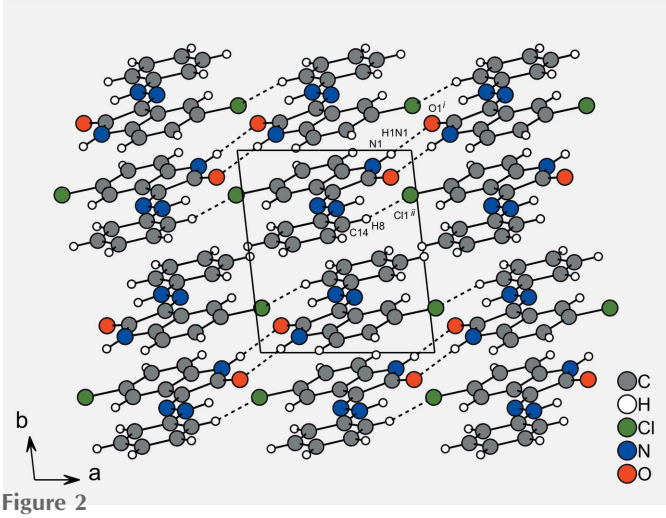


Figure 2
A packing diagram of the title compound, viewed along the *c* axis. Intermolecular N—H···O and C—H···Cl hydrogen bonds are shown as dashed lines. The planar hydrogen-bonded tapes are stacked along the *b* axis. Intramolecular N—H···O interactions are not shown for clarity.

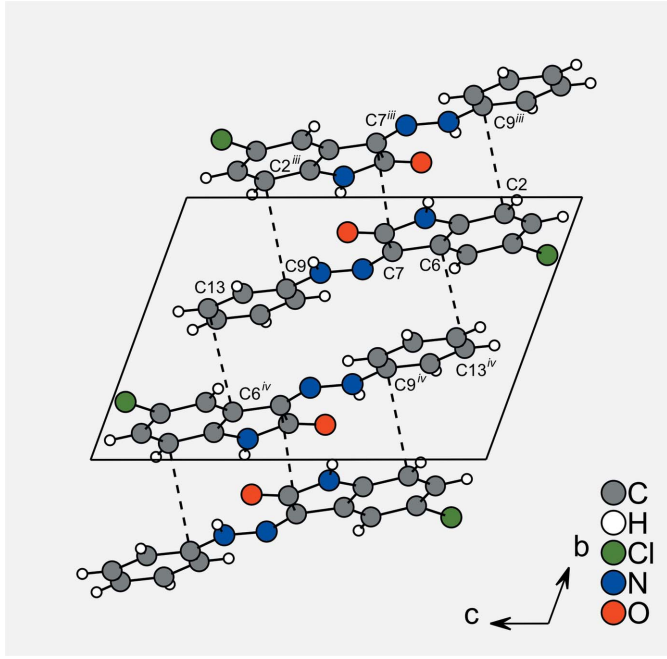


Figure 3
A packing diagram of the title compound, viewed along the *a* axis. The weak C···C contacts are shown as dashed lines. [Symmetry codes: (iii) $-x+1, -y+2, -z+1$; (iv) $-x+1, -y+1, -z+1$.]

of the enzyme was obtained from Protein Data Bank (PDB ID: 1ZXM; Wei *et al.*, 2005). Intermolecular interactions between the isatin–hydrazone derivative and the DNA topoisomerase IIα were found with the lowest binding energy score after 50 RBO cycles (Rigid-Body Optimization). The selected nonbonding interactions are H1*N1*···O (SER320) = 2.4849 Å, O*E1* (GLN309)···Cl1 = 2.5168 Å, O (GLN310)···*Cg*1 = 2.18535 Å and C*G2* (ILE311)···*Cg*2 = 3.58398 Å, where *Cg*1 and *Cg*2 are the centroids of the pyrrole aromatic ring and the terminal phenyl ring, respectively (Fig. 4). The global free energy of −26.59 kJ mol^{-1} was found for the 5-chloroisatine-3-phenylhydrazone/DNA topoisomerase IIα interaction. After the refinement, the top-ranked conformation was analysed using the *Discovery Studio Modeling Environment* software (Accelrys Software, 2013). The results of the

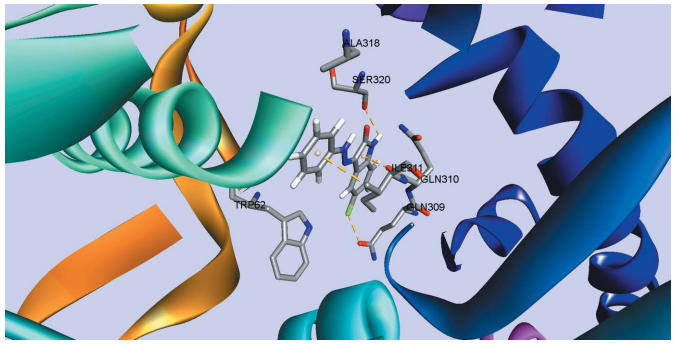


Figure 4
Intermolecular interactions between the title compound and the DNA topoisomerase IIα enzyme. The interactions are shown as yellow dashed lines and the figure is simplified for clarity.

evaluation agree with literature data for molecular docking and cytotoxic activity of hydrazone derivatives against breast cancer cells (Dandawate *et al.*, 2012).

Synthesis and crystallization

All starting materials are commercially available and were used without further purification. The synthesis was adapted from a procedure reported previously (Hajare *et al.*, 2009; Fonseca *et al.*, 2011). The glacial acetic acid catalyzed reaction of 5-chloroisatin (3 mmol) and phenylhydrazine (3 mmol) in methanol (40 ml) was refluxed for 4 h. After cooling and filtering, single crystals suitable for X-ray diffraction were obtained.

Refinement

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{14}H_{10}ClN_3O$
M_r	271.70
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	200
a, b, c (Å)	6.8759 (4), 8.2563 (5), 12.0403 (7)
α, β, γ (°)	109.156 (2), 103.979 (2), 91.485 (2)
V (Å^3)	622.41 (6)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.30
Crystal size (mm)	0.40 × 0.18 × 0.02
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2013)
T_{min}, T_{max}	0.706, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14457, 3638, 2877
R_{int}	0.021
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.705
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.035, 0.104, 1.09
No. of reflections	3638
No. of parameters	172
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.39, −0.21

Computer programs: *APEX2* (Bruker, 2013), *SAINT* (Bruker, 2013), *SHELXS97* (Sheldrick, 2008), *SHELXL97* (Sheldrick, 2008), *DIAMOND* (Brandenburg, 2006), *publCIF* (Westrip, 2010), *enCIFer* (Allen *et al.*, 2004).

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full crystallographic data

IUCrData (2016). **1**, x160258 [https://doi.org/10.1107/S2414314616002583]

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Crystal data

$C_{14}H_{10}ClN_3O$
$M_r = 271.70$
Triclinic, $P\overline{1}$
$a = 6.8759$ (4) Å
$b = 8.2563$ (5) Å
$c = 12.0403$ (7) Å
$\alpha = 109.156$ (2)°
$\beta = 103.979$ (2)°
$\gamma = 91.485$ (2)°
$V = 622.41$ (6) Å^3
$Z = 2$
$F(000) = 280$
$D_x = 1.450$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6679 reflections
$\theta = 2.6$–$30.0°$
$\mu = 0.30$ mm^{-1}
$T = 200$ K
Plate, yellow
0.40 × 0.18 × 0.02 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube, Bruker APEXII
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2013)
$T_{min} = 0.706$, $T_{max} = 0.746$
14457 measured reflections
3638 independent reflections
2877 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 30.1°$, $\theta_{min} = 1.9°$
$h = -9 \rightarrow 9$
$k = -11 \rightarrow 11$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.104$
$S = 1.09$
3638 reflections
172 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
$w = 1/[\sigma^2(F_o^2) + (0.0597P)^2 + 0.0323P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.39$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ 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.

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}
C1	0.58736 (15)	0.89630 (14)	0.28628 (10)	0.0247 (2)
C2	0.55505 (17)	0.93700 (15)	0.18143 (11)	0.0296 (2)
H1	0.6619	0.9890	0.1627	0.036*
C3	0.36025 (18)	0.89929 (16)	0.10383 (11)	0.0322 (3)
H2	0.3329	0.9255	0.0308	0.039*
C4	0.20611 (17)	0.82329 (16)	0.13323 (11)	0.0305 (2)
C5	0.23752 (16)	0.78126 (15)	0.23827 (10)	0.0277 (2)
H3	0.1304	0.7292	0.2567	0.033*
C6	0.43115 (15)	0.81814 (13)	0.31527 (10)	0.0239 (2)
C7	0.51991 (15)	0.79309 (13)	0.42956 (10)	0.0238 (2)
C8	0.73649 (15)	0.86214 (14)	0.46652 (10)	0.0254 (2)
C9	0.43396 (16)	0.65136 (14)	0.66321 (10)	0.0250 (2)
C10	0.22536 (17)	0.61127 (16)	0.63139 (11)	0.0319 (3)
H4	0.1434	0.6236	0.5595	0.038*
C11	0.1392 (2)	0.55320 (18)	0.70614 (13)	0.0402 (3)
H5	−0.0029	0.5250	0.6847	0.048*
C12	0.2568 (2)	0.53545 (18)	0.81179 (12)	0.0392 (3)
H6	0.1959	0.4954	0.8623	0.047*
C13	0.4635 (2)	0.57654 (17)	0.84283 (11)	0.0366 (3)
H7	0.5447	0.5653	0.9153	0.044*
C14	0.55336 (18)	0.63397 (15)	0.76915 (11)	0.0305 (2)
H8	0.6956	0.6613	0.7907	0.037*
Cl1	−0.03571 (5)	0.77931 (5)	0.03465 (3)	0.04731 (12)
N3	0.53041 (13)	0.71228 (12)	0.59226 (8)	0.0268 (2)
H1N3	0.6698	0.7526	0.6194	0.040*
N1	0.76714 (13)	0.92054 (13)	0.37801 (9)	0.0279 (2)
H1N1	0.8812	0.9812	0.3846	0.042*
N2	0.42461 (13)	0.72598 (11)	0.48848 (8)	0.0249 (2)
O1	0.86352 (11)	0.86715 (11)	0.56087 (8)	0.0320 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0212 (5)	0.0253 (5)	0.0263 (5)	0.0014 (4)	0.0054 (4)	0.0079 (4)
C2	0.0292 (5)	0.0334 (6)	0.0288 (5)	0.0011 (4)	0.0098 (4)	0.0126 (5)
C3	0.0340 (6)	0.0381 (6)	0.0260 (5)	0.0045 (5)	0.0065 (5)	0.0140 (5)

C4	0.0249 (5)	0.0373 (6)	0.0271 (5)	0.0040 (4)	0.0024 (4)	0.0115 (5)
C5	0.0221 (5)	0.0320 (6)	0.0278 (5)	0.0002 (4)	0.0037 (4)	0.0108 (4)
C6	0.0218 (5)	0.0242 (5)	0.0252 (5)	0.0015 (4)	0.0055 (4)	0.0087 (4)
C7	0.0200 (4)	0.0245 (5)	0.0254 (5)	0.0006 (4)	0.0035 (4)	0.0085 (4)
C8	0.0207 (5)	0.0256 (5)	0.0286 (5)	0.0006 (4)	0.0042 (4)	0.0096 (4)
C9	0.0264 (5)	0.0221 (5)	0.0250 (5)	0.0004 (4)	0.0051 (4)	0.0074 (4)
C10	0.0269 (5)	0.0373 (6)	0.0318 (6)	−0.0005 (5)	0.0035 (4)	0.0157 (5)
C11	0.0317 (6)	0.0489 (8)	0.0420 (7)	−0.0041 (5)	0.0112 (5)	0.0179 (6)
C12	0.0457 (7)	0.0412 (7)	0.0348 (6)	−0.0031 (6)	0.0150 (6)	0.0159 (5)
C13	0.0455 (7)	0.0378 (7)	0.0264 (6)	0.0021 (5)	0.0054 (5)	0.0142 (5)
C14	0.0290 (5)	0.0330 (6)	0.0275 (5)	0.0010 (4)	0.0026 (4)	0.0114 (5)
Cl1	0.02844 (16)	0.0736 (3)	0.03773 (19)	0.00142 (15)	−0.00409 (12)	0.02592 (17)
N3	0.0215 (4)	0.0317 (5)	0.0263 (5)	−0.0017 (3)	0.0014 (3)	0.0128 (4)
N1	0.0200 (4)	0.0341 (5)	0.0293 (5)	−0.0020 (4)	0.0042 (3)	0.0126 (4)
N2	0.0233 (4)	0.0258 (5)	0.0244 (4)	0.0004 (3)	0.0032 (3)	0.0096 (4)
O1	0.0216 (4)	0.0400 (5)	0.0331 (4)	−0.0018 (3)	−0.0001 (3)	0.0165 (4)

Geometric parameters (Å, º)

C1—C2	1.3794 (16)	C9—C10	1.3929 (15)
C1—N1	1.4038 (13)	C9—C14	1.3935 (15)
C1—C6	1.4089 (14)	C9—N3	1.4004 (14)
C2—C3	1.3953 (16)	C10—C11	1.3844 (17)
C2—H1	0.9500	C10—H4	0.9500
C3—C4	1.3910 (17)	C11—C12	1.3874 (18)
C3—H2	0.9500	C11—H5	0.9500
C4—C5	1.3880 (16)	C12—C13	1.3819 (19)
C4—Cl1	1.7429 (11)	C12—H6	0.9500
C5—C6	1.3864 (14)	C13—C14	1.3853 (17)
C5—H3	0.9500	C13—H7	0.9500
C6—C7	1.4479 (15)	C14—H8	0.9500
C7—N2	1.3051 (13)	N3—N2	1.3271 (12)
C7—C8	1.4866 (14)	N3—H1N3	0.9470
C8—O1	1.2422 (13)	N1—H1N1	0.8924
C8—N1	1.3613 (14)		
C2—C1—N1	128.82 (10)	C10—C9—N3	121.88 (10)
C2—C1—C6	121.93 (10)	C14—C9—N3	117.84 (10)
N1—C1—C6	109.24 (9)	C11—C10—C9	119.00 (11)
C1—C2—C3	117.80 (10)	C11—C10—H4	120.5
C1—C2—H1	121.1	C9—C10—H4	120.5
C3—C2—H1	121.1	C10—C11—C12	121.15 (12)
C4—C3—C2	120.09 (10)	C10—C11—H5	119.4
C4—C3—H2	120.0	C12—C11—H5	119.4
C2—C3—H2	120.0	C13—C12—C11	119.36 (12)
C5—C4—C3	122.47 (10)	C13—C12—H6	120.3
C5—C4—Cl1	118.70 (9)	C11—C12—H6	120.3
C3—C4—Cl1	118.83 (9)	C12—C13—C14	120.57 (11)

C6—C5—C4	117.51 (10)	C12—C13—H7	119.7
C6—C5—H3	121.2	C14—C13—H7	119.7
C4—C5—H3	121.2	C13—C14—C9	119.65 (11)
C5—C6—C1	120.19 (10)	C13—C14—H8	120.2
C5—C6—C7	133.19 (10)	C9—C14—H8	120.2
C1—C6—C7	106.62 (9)	N2—N3—C9	120.29 (9)
N2—C7—C6	125.89 (9)	N2—N3—H1N3	118.1
N2—C7—C8	127.52 (10)	C9—N3—H1N3	121.4
C6—C7—C8	106.58 (9)	C8—N1—C1	110.82 (9)
O1—C8—N1	126.93 (10)	C8—N1—H1N1	123.5
O1—C8—C7	126.34 (10)	C1—N1—H1N1	124.9
N1—C8—C7	106.73 (9)	C7—N2—N3	117.79 (9)
C10—C9—C14	120.27 (10)		

N1—C1—C2—C3	179.90 (11)	N2—C7—C8—N1	−179.18 (11)
C6—C1—C2—C3	0.42 (17)	C6—C7—C8—N1	−0.52 (12)
C1—C2—C3—C4	0.07 (18)	C14—C9—C10—C11	−0.35 (18)
C2—C3—C4—C5	−0.35 (19)	N3—C9—C10—C11	−179.38 (11)
C2—C3—C4—Cl1	179.58 (9)	C9—C10—C11—C12	0.4 (2)
C3—C4—C5—C6	0.14 (17)	C10—C11—C12—C13	0.0 (2)
Cl1—C4—C5—C6	−179.80 (9)	C11—C12—C13—C14	−0.4 (2)
C4—C5—C6—C1	0.34 (16)	C12—C13—C14—C9	0.38 (19)
C4—C5—C6—C7	−179.66 (11)	C10—C9—C14—C13	−0.01 (18)
C2—C1—C6—C5	−0.64 (17)	N3—C9—C14—C13	179.05 (11)
N1—C1—C6—C5	179.79 (10)	C10—C9—N3—N2	−3.13 (16)
C2—C1—C6—C7	179.36 (10)	C14—C9—N3—N2	177.82 (10)
N1—C1—C6—C7	−0.21 (12)	O1—C8—N1—C1	−178.77 (11)
C5—C6—C7—N2	−0.9 (2)	C7—C8—N1—C1	0.40 (12)
C1—C6—C7—N2	179.13 (10)	C2—C1—N1—C8	−179.66 (11)
C5—C6—C7—C8	−179.56 (11)	C6—C1—N1—C8	−0.13 (13)
C1—C6—C7—C8	0.44 (12)	C6—C7—N2—N3	179.80 (10)
N2—C7—C8—O1	0.00 (19)	C8—C7—N2—N3	−1.79 (17)
C6—C7—C8—O1	178.66 (11)	C9—N3—N2—C7	175.99 (10)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H1*N*3···O1	0.95	2.00	2.7581 (12)	136
N1—H1*N*1···O1^{i}	0.89	1.97	2.8431 (12)	167
C14—H8···Cl1^{ii}	0.95	2.90	3.5476 (12)	127

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