IUCrData

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1-[(7*E*)-7-(2-Chlorobenzylidene)-3-(2-chlorophenyl)-3,3a,4,5,6,7-hexahydro-2*H*-indazol-2-yl]-ethanone

Farook Adam,[a]* Nadiah Ameram,[b] Seranthimata Samshuddin,[c] Kurady Akhilesh Bairy[d] and Madhugiri Shivashankarappa Sunil[d]

[a]School of Chemical Sciences, Unibersiti Science Malaysia, 11800, Minden, Pulau Pinang., Malaysia, [b]School of Chemical Sciences, Universiti Science Malaysia, 11800, Minden, Pulau Pinang., Malaysia, [c]Department of P.G. Studies in Chemistry, Alva's College, Moodbidri, Karnataka 574 227, India, and [d]Department of Chemistry, SDM Institute of Technology, Ujire, Karnataka 574 240, India. *Correspondence e-mail: farook@usm.my

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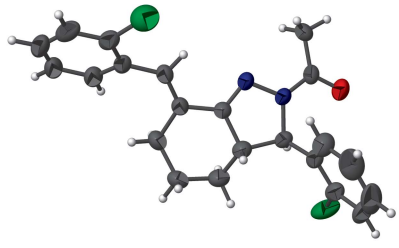
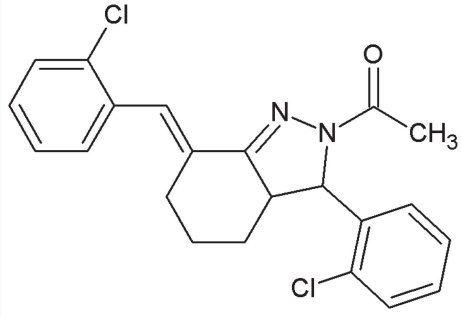
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{22}H_{20}Cl_2N_2O$, the diazole ring adopts a shallow envelope conformation with the methine C atom bonded to the adjacent chlorobenzene ring as the flap. The dihedral angles between the heterocyclic ring and the pendant chlorobenzene rings are 61.4 (2) and 80.3 (2)°. In the crystal, weak C—H···Cl interactions connect the molecules into [001] chains.

3D view



Chemical scheme



Structure description

Heterocycles containing 1,2-diazole systems such as indazole have attracted much attention for the design and synthesis of novel biologically active agents. They display various biological activities such as analgesic, anti inflammatory, anti-depressant, anti-tumor, anti-hypertensive, anti-viral and anti-cancer activities (Jain *et al.*, 1987; Palazzo *et al.*, 1966; Popat *et al.*, 2003).

The crystal structure of an indazole derivative, *viz*., 4,6-bis(4-fluorophenyl)-2-phenyl-1*H*-indazol-3(2*H*)-one (Butcher *et al.*, 2011) has been reported. As part of our studies in this area, the title compound (I) was synthesized and its crystal structure is reported here (Fig. 1). The 1,2-diazole ring adopts a shallow envelope conformation, with C14 as the flap; the dihedral angles between this ring (all atoms) and the C6 and C15 chlorobenzene rings are 61.4 (2) and 80.3 (2)°, respectively. The cyclohexyl ring adopts a distorted chair conformation. In the crystal, weak C—H···Cl interactions (Table 1 and (Fig. 2)) connect the molecules into [001] chains.

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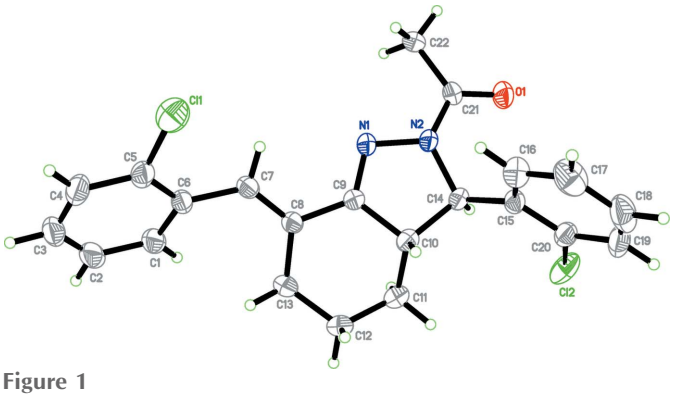

Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids.

Synthesis and crystallization

A mixture of 2,6-bis(2-chlorobenzylidene)cyclohexanone (3.43 g, 0.01 mol) and hydrazine hydrate (1 ml) in 30 ml acetic acid was refluxed for 10 h. The reaction mixture was cooled and poured into 50 ml ice-cold water. The precipitate was collected by filtration and purified by recrystallization from ethanol. Colourless plates were grown from DMF solution by slow evaporation; Yield: 72% (m.p. 458 K).

Refinement

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

Acknowledgements

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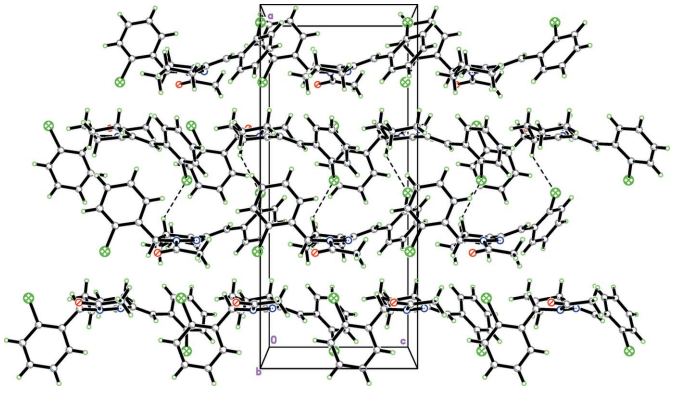

Figure 2
The crystal packing of (I), viewed down the *b* axis, showing the formation of [001] chains linked by C—H···Cl interactions (dashed lines).

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10*A*···Cl1^{i}	1.00	2.85	3.677 (4)	140

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{22}H_{20}Cl_2N_2O$
M_r	399.30
Crystal system, space group	Orthorhombic, $Pca2_1$
Temperature (K)	100
a, *b*, *c* (Å)	20.9334 (17), 10.2009 (8), 9.0493 (7)
V (Å^3)	1932.4 (3)
Z	4
Radiation type	Mo *Kα*
μ (mm^{-1})	0.35
Crystal size (mm)	0.64 × 0.25 × 0.09
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)
T_{min}, T_{max}	0.653, 0.855
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	38855, 3549, 2966
R_{int}	0.058
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.605
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.041, 0.094, 1.05
No. of reflections	3549
No. of parameters	245
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.14, −0.16
Absolute structure	Flack *x* determined using 1138 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.05 (3)

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXS97* and *SHELXTL* (Sheldrick 2008) and *SHELXL2014* (Sheldrick, 2015).

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full crystallographic data

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Crystal data

$C_{22}H_{20}Cl_2N_2O$
M_r = 399.30
Orthorhombic, $Pca2_1$
a = 20.9334 (17) Å
b = 10.2009 (8) Å
c = 9.0493 (7) Å
V = 1932.4 (3) Å^3
Z = 4
$F(000)$ = 832
D_x = 1.373 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9969 reflections
θ = 2.2–30.1°
μ = 0.35 mm^{-1}
T = 100 K
Plate, colourless
0.64 × 0.25 × 0.09 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.653, T_{max} = 0.855
38855 measured reflections
3549 independent reflections
2966 reflections with $I > 2\sigma(I)$
R_{int} = 0.058
θ_{max} = 25.5°, θ_{min} = 2.0°
h = −25→25
k = −11→12
l = −10→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.094
S = 1.05
3549 reflections
245 parameters
1 restraint
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0448P)^2 + 0.3258P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Absolute structure: Flack x determined using 1138 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.05 (3)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.48134 (5)	0.51064 (11)	0.96839 (15)	0.0795 (3)
Cl2	0.31606 (5)	0.76773 (13)	−0.03357 (12)	0.0821 (4)
O1	0.31810 (15)	1.0071 (3)	0.3493 (3)	0.0653 (7)
N1	0.34670 (14)	0.7266 (3)	0.5626 (3)	0.0459 (7)
N2	0.34748 (13)	0.8138 (2)	0.4423 (3)	0.0472 (7)
C1	0.3342 (2)	0.2839 (4)	0.8519 (5)	0.0616 (10)
H1A	0.2995	0.2839	0.7840	0.074*
C2	0.3395 (3)	0.1818 (4)	0.9532 (6)	0.0805 (14)
H2A	0.3086	0.1137	0.9540	0.097*
C3	0.3891 (3)	0.1791 (5)	1.0515 (5)	0.0892 (17)
H3A	0.3933	0.1078	1.1184	0.107*
C4	0.4327 (3)	0.2793 (5)	1.0535 (4)	0.0763 (13)
H4A	0.4670	0.2783	1.1223	0.092*
C5	0.42650 (17)	0.3825 (3)	0.9541 (4)	0.0556 (9)
C6	0.37857 (17)	0.3867 (3)	0.8475 (4)	0.0477 (8)
C7	0.37465 (17)	0.4943 (3)	0.7390 (4)	0.0455 (8)
H7A	0.3896	0.5772	0.7722	0.055*
C8	0.35296 (17)	0.4906 (3)	0.6007 (4)	0.0442 (8)
C9	0.35321 (16)	0.6102 (3)	0.5097 (3)	0.0421 (8)
C10	0.36092 (17)	0.6037 (3)	0.3445 (4)	0.0482 (8)
H10A	0.4069	0.5846	0.3235	0.058*
C11	0.3220 (2)	0.4941 (4)	0.2782 (4)	0.0621 (10)
H11A	0.3306	0.4870	0.1710	0.074*
H11B	0.2758	0.5113	0.2922	0.074*
C12	0.3409 (2)	0.3679 (4)	0.3562 (5)	0.0616 (11)
H12A	0.3871	0.3521	0.3403	0.074*
H12B	0.3172	0.2939	0.3114	0.074*
C13	0.3275 (2)	0.3709 (4)	0.5217 (4)	0.0609 (11)
H13A	0.2807	0.3664	0.5371	0.073*
H13B	0.3466	0.2918	0.5673	0.073*
C14	0.34787 (17)	0.7469 (3)	0.2968 (3)	0.0448 (8)
H14A	0.3049	0.7538	0.2490	0.054*
C15	0.39886 (17)	0.7980 (3)	0.1944 (4)	0.0452 (8)
C16	0.4588 (2)	0.8303 (4)	0.2481 (5)	0.0662 (11)
H16A	0.4665	0.8261	0.3514	0.079*
C17	0.5079 (2)	0.8686 (5)	0.1552 (7)	0.0863 (15)
H17A	0.5487	0.8896	0.1944	0.104*
C18	0.4970 (3)	0.8760 (5)	0.0047 (6)	0.0880 (17)
H18A	0.5305	0.9017	−0.0599	0.106*
C19	0.4382 (2)	0.8463 (4)	−0.0511 (5)	0.0725 (12)
H19A	0.4307	0.8521	−0.1544	0.087*
C20	0.38947 (19)	0.8077 (3)	0.0429 (4)	0.0534 (9)
C21	0.32633 (15)	0.9393 (3)	0.4583 (4)	0.0478 (7)
C22	0.3155 (2)	0.9878 (3)	0.6132 (4)	0.0566 (10)
H22A	0.3542	0.9736	0.6721	0.085*

H22B	0.2798	0.9399	0.6578	0.085*
H22C	0.3055	1.0817	0.6109	0.085*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0679 (6)	0.0959 (8)	0.0747 (7)	0.0049 (5)	−0.0093 (6)	−0.0008 (7)
Cl2	0.0839 (7)	0.1218 (9)	0.0406 (5)	0.0197 (6)	−0.0111 (5)	−0.0060 (6)
O1	0.094 (2)	0.0515 (15)	0.0506 (15)	0.0111 (14)	0.0028 (15)	0.0149 (13)
N1	0.0627 (18)	0.0390 (16)	0.0360 (14)	0.0033 (14)	0.0002 (13)	0.0064 (13)
N2	0.0714 (18)	0.0385 (14)	0.0317 (14)	0.0053 (12)	0.0014 (14)	0.0054 (12)
C1	0.082 (3)	0.049 (2)	0.054 (2)	−0.004 (2)	0.021 (2)	0.0027 (19)
C2	0.133 (4)	0.047 (2)	0.061 (3)	−0.005 (2)	0.039 (3)	0.004 (2)
C3	0.161 (5)	0.052 (3)	0.055 (3)	0.023 (3)	0.032 (3)	0.015 (2)
C4	0.112 (4)	0.075 (3)	0.042 (2)	0.040 (3)	0.007 (2)	0.007 (2)
C5	0.070 (2)	0.054 (2)	0.0430 (18)	0.0180 (16)	0.011 (2)	0.0028 (19)
C6	0.061 (2)	0.0409 (19)	0.0413 (18)	0.0114 (16)	0.0148 (18)	0.0039 (15)
C7	0.053 (2)	0.0350 (17)	0.0482 (18)	0.0012 (15)	0.0052 (16)	0.0012 (15)
C8	0.053 (2)	0.0371 (18)	0.043 (2)	0.0014 (15)	0.0071 (16)	0.0004 (15)
C9	0.0513 (19)	0.0380 (19)	0.0370 (17)	0.0011 (15)	0.0018 (14)	−0.0011 (14)
C10	0.056 (2)	0.050 (2)	0.0391 (17)	0.0023 (16)	0.0019 (16)	−0.0013 (15)
C11	0.083 (3)	0.059 (2)	0.0438 (19)	−0.004 (2)	0.0000 (19)	−0.0081 (19)
C12	0.083 (3)	0.048 (2)	0.053 (2)	−0.004 (2)	0.005 (2)	−0.0122 (18)
C13	0.087 (3)	0.039 (2)	0.057 (2)	−0.0069 (19)	0.007 (2)	−0.0037 (17)
C14	0.057 (2)	0.046 (2)	0.0321 (17)	0.0020 (15)	0.0006 (16)	0.0020 (15)
C15	0.053 (2)	0.0418 (18)	0.0402 (17)	0.0076 (16)	0.0014 (16)	0.0065 (15)
C16	0.068 (3)	0.070 (3)	0.060 (2)	−0.001 (2)	0.001 (2)	0.009 (2)
C17	0.062 (3)	0.080 (3)	0.117 (5)	−0.008 (2)	0.015 (3)	0.009 (3)
C18	0.089 (4)	0.070 (3)	0.105 (4)	0.007 (3)	0.047 (3)	0.026 (3)
C19	0.094 (3)	0.069 (3)	0.054 (2)	0.018 (2)	0.029 (2)	0.018 (2)
C20	0.068 (2)	0.049 (2)	0.0424 (19)	0.0176 (18)	0.0053 (18)	0.0045 (16)
C21	0.0599 (19)	0.0390 (17)	0.0445 (18)	−0.0028 (15)	−0.0008 (19)	0.0078 (18)
C22	0.084 (3)	0.0365 (18)	0.049 (2)	0.0012 (18)	0.000 (2)	−0.0046 (17)

Geometric parameters (Å, º)

Cl1—C5	1.744 (4)	C10—H10A	1.0000
Cl2—C20	1.734 (4)	C11—C12	1.521 (6)
O1—C21	1.218 (4)	C11—H11A	0.9900
N1—C9	1.287 (4)	C11—H11B	0.9900
N1—N2	1.406 (4)	C12—C13	1.525 (5)
N2—C21	1.363 (4)	C12—H12A	0.9900
N2—C14	1.483 (4)	C12—H12B	0.9900
C1—C2	1.392 (6)	C13—H13A	0.9900
C1—C6	1.402 (5)	C13—H13B	0.9900
C1—H1A	0.9500	C14—C15	1.506 (5)
C2—C3	1.368 (7)	C14—H14A	1.0000
C2—H2A	0.9500	C15—C16	1.386 (5)

C3—C4	1.371 (7)	C15—C20	1.389 (5)
C3—H3A	0.9500	C16—C17	1.383 (6)
C4—C5	1.391 (5)	C16—H16A	0.9500
C4—H4A	0.9500	C17—C18	1.383 (7)
C5—C6	1.392 (5)	C17—H17A	0.9500
C6—C7	1.475 (5)	C18—C19	1.365 (7)
C7—C8	1.332 (5)	C18—H18A	0.9500
C7—H7A	0.9500	C19—C20	1.385 (5)
C8—C9	1.472 (5)	C19—H19A	0.9500
C8—C13	1.512 (5)	C21—C22	1.504 (5)
C9—C10	1.505 (5)	C22—H22A	0.9800
C10—C11	1.508 (5)	C22—H22B	0.9800
C10—C14	1.547 (5)	C22—H22C	0.9800
C9—N1—N2	107.2 (3)	C11—C12—H12A	109.0
C21—N2—N1	120.6 (3)	C13—C12—H12A	109.0
C21—N2—C14	121.9 (3)	C11—C12—H12B	109.0
N1—N2—C14	113.3 (2)	C13—C12—H12B	109.0
C2—C1—C6	121.7 (5)	H12A—C12—H12B	107.8
C2—C1—H1A	119.2	C8—C13—C12	114.6 (3)
C6—C1—H1A	119.2	C8—C13—H13A	108.6
C3—C2—C1	120.3 (4)	C12—C13—H13A	108.6
C3—C2—H2A	119.8	C8—C13—H13B	108.6
C1—C2—H2A	119.8	C12—C13—H13B	108.6
C2—C3—C4	119.9 (4)	H13A—C13—H13B	107.6
C2—C3—H3A	120.1	N2—C14—C15	113.0 (3)
C4—C3—H3A	120.1	N2—C14—C10	100.8 (2)
C3—C4—C5	119.6 (5)	C15—C14—C10	111.9 (3)
C3—C4—H4A	120.2	N2—C14—H14A	110.3
C5—C4—H4A	120.2	C15—C14—H14A	110.3
C4—C5—C6	122.6 (4)	C10—C14—H14A	110.3
C4—C5—Cl1	117.2 (4)	C16—C15—C20	117.2 (3)
C6—C5—Cl1	120.2 (3)	C16—C15—C14	120.6 (3)
C5—C6—C1	115.8 (3)	C20—C15—C14	122.1 (3)
C5—C6—C7	121.6 (3)	C17—C16—C15	121.8 (4)
C1—C6—C7	122.6 (3)	C17—C16—H16A	119.1
C8—C7—C6	128.6 (3)	C15—C16—H16A	119.1
C8—C7—H7A	115.7	C18—C17—C16	119.5 (5)
C6—C7—H7A	115.7	C18—C17—H17A	120.2
C7—C8—C9	120.1 (3)	C16—C17—H17A	120.2
C7—C8—C13	126.0 (3)	C19—C18—C17	120.0 (4)
C9—C8—C13	114.0 (3)	C19—C18—H18A	120.0
N1—C9—C8	123.8 (3)	C17—C18—H18A	120.0
N1—C9—C10	114.9 (3)	C18—C19—C20	120.1 (4)
C8—C9—C10	121.3 (3)	C18—C19—H19A	120.0
C9—C10—C11	111.7 (3)	C20—C19—H19A	120.0
C9—C10—C14	102.5 (3)	C19—C20—C15	121.5 (4)
C11—C10—C14	119.6 (3)	C19—C20—Cl2	118.3 (3)

C9—C10—H10A	107.5	C15—C20—Cl2	120.2 (3)
C11—C10—H10A	107.5	O1—C21—N2	119.6 (3)
C14—C10—H10A	107.5	O1—C21—C22	123.2 (3)
C10—C11—C12	107.6 (3)	N2—C21—C22	117.2 (3)
C10—C11—H11A	110.2	C21—C22—H22A	109.5
C12—C11—H11A	110.2	C21—C22—H22B	109.5
C10—C11—H11B	110.2	H22A—C22—H22B	109.5
C12—C11—H11B	110.2	C21—C22—H22C	109.5
H11A—C11—H11B	108.5	H22A—C22—H22C	109.5
C11—C12—C13	113.0 (3)	H22B—C22—H22C	109.5

C9—N1—N2—C21	164.0 (3)	C7—C8—C13—C12	−146.9 (4)
C9—N1—N2—C14	6.5 (4)	C9—C8—C13—C12	32.2 (5)
C6—C1—C2—C3	−0.3 (6)	C11—C12—C13—C8	−50.2 (5)
C1—C2—C3—C4	1.9 (6)	C21—N2—C14—C15	72.4 (4)
C2—C3—C4—C5	−0.7 (6)	N1—N2—C14—C15	−130.5 (3)
C3—C4—C5—C6	−2.3 (6)	C21—N2—C14—C10	−168.0 (3)
C3—C4—C5—Cl1	177.0 (3)	N1—N2—C14—C10	−10.9 (3)
C4—C5—C6—C1	3.8 (5)	C9—C10—C14—N2	10.3 (3)
Cl1—C5—C6—C1	−175.6 (3)	C11—C10—C14—N2	134.5 (3)
C4—C5—C6—C7	−177.2 (3)	C9—C10—C14—C15	130.7 (3)
Cl1—C5—C6—C7	3.5 (4)	C11—C10—C14—C15	−105.1 (4)
C2—C1—C6—C5	−2.4 (5)	N2—C14—C15—C16	39.2 (4)
C2—C1—C6—C7	178.6 (4)	C10—C14—C15—C16	−73.8 (4)
C5—C6—C7—C8	148.7 (4)	N2—C14—C15—C20	−144.6 (3)
C1—C6—C7—C8	−32.4 (6)	C10—C14—C15—C20	102.4 (4)
C6—C7—C8—C9	−180.0 (3)	C20—C15—C16—C17	−1.1 (6)
C6—C7—C8—C13	−0.8 (6)	C14—C15—C16—C17	175.4 (4)
N2—N1—C9—C8	−178.2 (3)	C15—C16—C17—C18	0.5 (7)
N2—N1—C9—C10	1.4 (4)	C16—C17—C18—C19	0.3 (7)
C7—C8—C9—N1	−30.8 (5)	C17—C18—C19—C20	−0.6 (7)
C13—C8—C9—N1	150.0 (4)	C18—C19—C20—C15	−0.1 (6)
C7—C8—C9—C10	149.6 (4)	C18—C19—C20—Cl2	−178.7 (3)
C13—C8—C9—C10	−29.7 (5)	C16—C15—C20—C19	0.9 (5)
N1—C9—C10—C11	−137.2 (3)	C14—C15—C20—C19	−175.5 (3)
C8—C9—C10—C11	42.4 (5)	C16—C15—C20—Cl2	179.5 (3)
N1—C9—C10—C14	−8.0 (4)	C14—C15—C20—Cl2	3.1 (5)
C8—C9—C10—C14	171.6 (3)	N1—N2—C21—O1	−168.8 (3)
C9—C10—C11—C12	−55.0 (4)	C14—N2—C21—O1	−13.3 (5)
C14—C10—C11—C12	−174.6 (3)	N1—N2—C21—C22	12.4 (4)
C10—C11—C12—C13	61.1 (5)	C14—N2—C21—C22	167.9 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10*A*···Cl1^{i}	1.00	2.85	3.677 (4)	140

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