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2-(4-Chlorophenyl)-3-{[(1*E*)-(4-chlorophenyl)methylene]amino}-2,3-dihydroquinazolin-4(1*H*)-one

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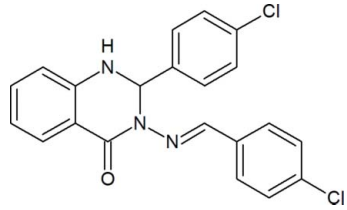
Key indicators: single-crystal X-ray study; T = 203 K; mean σ(C–C) = 0.002 Å; disorder in main residue; R factor = 0.045; wR factor = 0.055; data-to-parameter ratio = 25.0.

The title molecule, $C_{21}H_{15}Cl_2N_3O$, consists of two coplanar 4-chlorophenyl groups bonded to a distorted (envelope) dihydroquinazoline ring with a dihedral angle of 58.9 (1)° between the 4-chlorophenyl groups. The angles between the mean planes of the benzyl group of the nonplanar dihydroquinazoline group and those of the two 4-chlorophenyl groups are 82.0 (6) and 84.3 (3)°, respectively. The torsion angle of the methylene amine linkage indicates a significant twist between the dihydroquinazolin-4(1*H*)-one and attached 4-chlorophenyl group. Disordered chlorine atoms (0.86:0.14) occur within the singly attached 4-chlorophenyl group bonded to the dihydroquinazoline ring. Crystal packing is stabilized by intermolecular N—H···O hydrogen bonding between dihydroquinazoline groups, linking the molecules into chains along the *b* axis.

Related literature

For related structures, see: Shi *et al.* (2004*a*, 2004*b*); Shi, Li, Shi, Zhuang & Zhang (2004); Shi, Shi *et al.* (2004); Vembu *et al.* (2006); Swamy & Ravikumar (2005); Chruszcz *et al.* (2007). For related literature, see: Hodnett & Dunn (1970); Alaimo & Russel (1972); Alaimo & Hatton (1972); Cremer & Pople (1975); Misra *et al.* (1981); Varma *et al.* (1986); Singh & Dash (1988); Pandey *et al.* (1999); El-Masry *et al.* (2000); Desai *et al.* (2001); Birch *et al.* (2005).



Experimental

Crystal data

$C_{21}H_{15}Cl_2N_3O$
M_r = 396.26
Monoclinic, $P2_1/n$
a = 6.8774 (2) Å
b = 13.7315 (3) Å
c = 20.4667 (8) Å
β = 97.010 (3)°
V = 1918.36 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.35 mm^{-1}
T = 203 K
0.53 × 0.47 × 0.13 mm

Data collection

Oxford Diffraction Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.926, T_{max} = 1.000 (expected range = 0.885–0.955)
16112 measured reflections
6303 independent reflections
2674 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.055
S = 1.63
6303 reflections
252 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1^{i}	0.854 (12)	2.153 (13)	2.9877 (15)	165.7 (12)

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

Data collection: *CrysAlisPro* (Oxford Diffraction, 2007); cell refinement: *CrysAlisPro*; data reduction: *CrysAlisPro*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NC2054).

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supplementary materials

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2-(4-Chlorophenyl)-3-{[(1*E*)-(4-chlorophenyl)methylene]amino}-2,3-dihydroquinazolin-4(1*H*)-one

R. J. Butcher, J. P. Jasinski, B. Narayana, K. Sunil and H. S. Yathirajan

Comment

Substituted 2,3-dihydroquinazolin-4(1*H*)-ones are found to be potent inhibitors of inosine 5'-monophosphate dehydrogenase type II (Birch *et al.*, 2005) and also are found to possess antibacterial (Alaimo & Russel, 1972) and anthelmentic activities (Alaimo & Hatton, 1972). Schiff bases are used as substrates in the preparation of number of industrial and biologically active compounds *via* ring closure, cycloaddition and replacement reactions. Some Schiff base derivatives were reported to possess antimicrobial, anti-inflammatory and central nervous system activities. Moreover, Schiff bases are also known to have biological activities such as antimicrobial (El-Masry *et al.*, 2000; Pandey *et al.*, 1999), antifungal (Singh & Dash, 1988; Varma *et al.*, 1986), antitumor (Hodnett & Dunn, 1970., Misra *et al.*, 1981; Desai *et al.*, 2001), and also act as herbicides. The crystal structures of 3-(4-bromophenyl)-2,2-dimethyl-2,3-dihydroquinazolin-4(1*H*)-one (Shi, Li, Shi, Zhuang & Zhang, 2004), 3-(4-chlorophenyl)-3,4-dihydroquinazolin-2(1*H*)-one (Shi *et al.*, 2004*a*), 6-chloro-3-(4-chlorophenyl)-3,4-dihydroquinazolin-2(1*H*)-one acetone hemisolvate (Shi *et al.*, 2004*b*), 7-chloro-2,2-dimethyl-3-(4-methylphenyl)-1,2-dihydroquinazolin-4(3*H*)-one (Shi, Shi *et al.*, 2004), 2-(4-hydroxy-3-methoxyphenyl)-1-phenethyl-1,2-dihydroquinazolin-4(3*H*)-one (Swamy & Ravikumar, 2005), 5-chloro-3-hydroxy-2,2-dimethyl-2,3-dihydroquinazolin-4(1*H*)-one (Vembu *et al.*, 2006) and 2-(biphenyl-4-yl)-2,3-dihydroquinazolin-4(1*H*)-one (Chruszcz *et al.*, 2007) have been reported. A new quinazolinone containing Schiff base, $C_{21}H_{15}C_{l2}N_3O$, has been synthesized and its crystal structure is reported. In our synthesis we expected the formation of 2-amino-N'-[(1E)-(4- chlorophenyl)methylene]benzohydrazide. Instead the aldehyde reacted with both primary amino groups and the cyclized form was created producing the title compound, (I).

The six-membered pyrimidin-4(1*H*)-one ring within the quinazoline group (C1—C2—C7—N1—C8—N2) is a distorted envleope with Cremer & Pople (1975) puckering parameters Q, θ and φ of 0.4372 (17) Å, 121.2 (2)° and 129.4 (2)°, respectively (Fig. 1). For an ideal envelope conformation, θ and φ are 54.7° and (60*n*)°, respectively. The angle between the mean planes of the two coplanar 4-chlorophenyl groups is 58.9 (1)°. The angles between the mean planes of the benzyl group of the nonplanar, dihydroquinazolin-4 group and those of the two 4-chlorophenyl groups are 82.0 (6) and 84.3 (3)%, respectively. The torsion angles of the methylene amine linkage [N3–N2–C1–C2 = 159.78 (13)° and N3–C15–C16–C21 = −165.29 (16)°] indicates a significant twist between the dihydroquinazolin-4(1*H*)-one and attached 4-chlorophenyl group. Crystal packing is stabilized by intermolecular N1—H1A···O1 hydrogen bonding between nearby dihydroquinazolin groups which link the molecules into chains along the *b* axis of the unit cell (Fig.2).

Experimental

A mixture of 2-aminobenzohydrazide (0.302 g, 0.002 mol) and 4-chlorobenzaldehyde (0.28 g, 0.002 mol) in 15 ml of absolute ethyl alcohol containing 2 drops of 4 *M* sulfuric acid was refluxed for about 3 h. On cooling, the solid separated was filtered and recrystallized from a solvent mixture (8:2) of ethyl acetate and DMF (m.p.: 466–468 K). Analysis found: C 63.52, H 3.76, N 10.49%; $C_{21}H_{15}Cl2N_3O$ requires: C 63.65, H 3.82, N 10.60%.

Refinement

The C—H atoms were positioned with idealized geometry and were refined isotropic with U_{eq}(H) = 1.2 U_{eq}(c) using a riding model with C—H = 0.94 Å for aromatic and C—H = 0.99 Å for methine H atoms. The N—H H atom was located in difference map and was refined isotopic with varying coordinates. One chlorine atom is disordered in two positions and was refined anisotropic using a split model (s.o.f. = 0.143 (3) and 0.857 (3)).

Figures

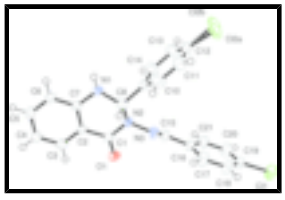

Fig. 1. Molecular structure of the title compound, showing atom labeling and 50% probability displacement ellipsoids.

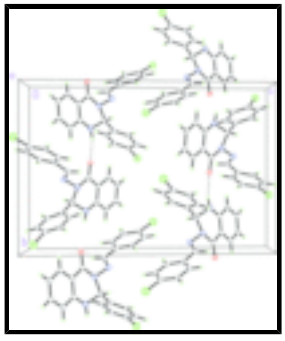

Fig. 2. Packing diagram for $C_{21}H_{15}Cl_2N_3O$ viewed down the *a* axis. Dashed lines indicate N—H···O intermolecular hydrogen bonds. Only the major component of the disordered chlorine atom (Cl2B) is displayed.

2-(4-Chlorophenyl)-3-{[(1E)-(4-chlorophenyl)methylene]amino}-2,3- dihydroquinazolin-4(1*H*)-one

Crystal data

$C_{21}H_{15}Cl_2N_3O$	F_{000} = 816
M_r = 396.26	D_x = 1.372 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 4254 reflections
a = 6.8774 (2) Å	θ = 4.7–32.5º
b = 13.7315 (3) Å	μ = 0.35 mm^{-1}
c = 20.4667 (8) Å	T = 203 K
β = 97.010 (3)º	Plate, colorless
V = 1918.36 (10) Å^3	0.53 × 0.47 × 0.13 mm
Z = 4	

Data collection

Oxford Diffraction Gemini diffractometer	2674 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.037

Monochromator: graphite
T = 203 K
φ and ω scans
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2007)
T_{min} = 0.926, T_{max} = 1.000
16112 measured reflections
6303 independent reflections

θ_{max} = 32.6º
θ_{min} = 4.7º
h = −10→10
k = −18→20
l = −29→30
Standard reflections: ?

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.055
S = 1.63
6303 reflections
252 parameters
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}
Extinction correction: none

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.

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 $F^2 > 2$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. A disordered chlorine atom, Cl2A [(0.143 (3)] & Cl2B [0.857 (3)], occurs within the singly attached 4-chlorophenyl group to the dihydroquinazolin-4 ring and was refined so that their occupancies summed to 1.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cl1	−0.10011 (6)	0.67297 (3)	1.01418 (2)	0.06572 (16)	
Cl2A	0.2071 (12)	0.0619 (3)	0.9802 (4)	0.0822 (5)	0.143 (3)
Cl2B	0.1030 (2)	0.06077 (5)	0.94734 (8)	0.0822 (5)	0.857 (3)
O1	0.65192 (12)	0.52725 (6)	0.74083 (5)	0.0381 (3)	
N1	0.74123 (16)	0.23816 (9)	0.75887 (6)	0.0327 (3)	
H1A	0.7714 (16)	0.1785 (9)	0.7664 (6)	0.034 (4)*	
N2	0.59892 (14)	0.38310 (7)	0.79096 (6)	0.0289 (3)	

N3	0.51282 (17)	0.43070 (8)	0.84227 (6)	0.0365 (3)
C1	0.68930 (18)	0.43957 (10)	0.74828 (7)	0.0302 (4)
C2	0.83198 (18)	0.38806 (9)	0.71214 (7)	0.0277 (3)
C3	0.94084 (19)	0.43931 (10)	0.67071 (7)	0.0392 (4)
H3A	0.9251	0.5071	0.6663	0.047*
C4	1.0717 (2)	0.39151 (11)	0.63603 (8)	0.0461 (5)
H4A	1.1477	0.4266	0.6089	0.055*
C5	1.09004 (19)	0.29123 (11)	0.64157 (8)	0.0438 (4)
H5A	1.1773	0.2583	0.6173	0.053*
C6	0.98294 (18)	0.23944 (10)	0.68187 (7)	0.0366 (4)
H6A	0.9965	0.1714	0.6849	0.044*
C7	0.85406 (18)	0.28752 (9)	0.71830 (7)	0.0290 (3)
C8	0.68991 (19)	0.28985 (9)	0.81588 (8)	0.0348 (4)
H8A	0.8092	0.3031	0.8468	0.042*
C9	0.5468 (2)	0.23071 (9)	0.84980 (8)	0.0311 (4)
C10	0.5939 (2)	0.19858 (10)	0.91276 (9)	0.0454 (4)
H10A	0.7185	0.2122	0.9351	0.055*
C11	0.4605 (3)	0.14606 (11)	0.94427 (9)	0.0576 (5)
H11A	0.4933	0.1247	0.9879	0.069*
C12	0.2817 (3)	0.12593 (11)	0.91110 (11)	0.0555 (5)
C13	0.2316 (2)	0.15577 (11)	0.84789 (11)	0.0562 (5)
H13A	0.1078	0.1407	0.8254	0.067*
C14	0.3658 (2)	0.20870 (10)	0.81721 (8)	0.0454 (4)
H14A	0.3326	0.2298	0.7736	0.055*
C15	0.3577 (2)	0.47659 (10)	0.82277 (8)	0.0366 (4)
H15A	0.3095	0.4768	0.7778	0.044*
C16	0.2520 (2)	0.52966 (9)	0.86972 (8)	0.0307 (4)
C17	0.3345 (2)	0.54820 (10)	0.93330 (8)	0.0425 (4)
H17A	0.4655	0.5304	0.9463	0.051*
C18	0.2287 (2)	0.59239 (10)	0.97826 (8)	0.0448 (4)
H18A	0.2860	0.6043	1.0216	0.054*
C19	0.0381 (2)	0.61862 (10)	0.95834 (9)	0.0394 (4)
C20	−0.0444 (2)	0.60432 (11)	0.89521 (9)	0.0514 (5)
H20A	−0.1738	0.6245	0.8819	0.062*
C21	0.0633 (2)	0.55979 (11)	0.85062 (8)	0.0464 (4)
H21A	0.0067	0.5501	0.8069	0.056*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0652 (3)	0.0591 (3)	0.0796 (4)	0.0083 (2)	0.0364 (3)	−0.0211 (3)
Cl2A	0.0861 (9)	0.0506 (3)	0.1259 (10)	−0.0030 (4)	0.0771 (8)	0.0145 (5)
Cl2B	0.0861 (9)	0.0506 (3)	0.1259 (10)	−0.0030 (4)	0.0771 (8)	0.0145 (5)
O1	0.0502 (6)	0.0192 (6)	0.0473 (7)	0.0034 (5)	0.0154 (5)	0.0021 (5)
N1	0.0446 (7)	0.0153 (7)	0.0414 (9)	0.0031 (6)	0.0183 (7)	−0.0006 (7)
N2	0.0390 (7)	0.0177 (6)	0.0323 (8)	0.0055 (5)	0.0138 (6)	0.0015 (6)
N3	0.0462 (8)	0.0272 (7)	0.0388 (9)	0.0043 (6)	0.0159 (7)	0.0001 (7)
C1	0.0365 (9)	0.0222 (8)	0.0316 (10)	−0.0041 (7)	0.0034 (8)	−0.0022 (8)

C2	0.0347 (8)	0.0186 (8)	0.0310 (9)	0.0002 (6)	0.0090 (7)	−0.0011 (7)
C3	0.0552 (10)	0.0225 (8)	0.0429 (11)	−0.0029 (8)	0.0178 (9)	0.0002 (8)
C4	0.0635 (11)	0.0322 (10)	0.0486 (12)	−0.0055 (8)	0.0310 (10)	0.0003 (9)
C5	0.0521 (10)	0.0361 (9)	0.0483 (12)	0.0003 (8)	0.0257 (9)	−0.0045 (9)
C6	0.0470 (9)	0.0213 (8)	0.0446 (11)	0.0027 (7)	0.0179 (9)	−0.0018 (8)
C7	0.0330 (8)	0.0233 (8)	0.0317 (10)	−0.0019 (7)	0.0083 (7)	0.0002 (8)
C8	0.0403 (9)	0.0241 (8)	0.0418 (11)	0.0034 (7)	0.0121 (8)	0.0034 (8)
C9	0.0378 (9)	0.0201 (8)	0.0373 (11)	0.0029 (7)	0.0125 (8)	0.0003 (8)
C10	0.0588 (10)	0.0349 (9)	0.0422 (12)	−0.0011 (8)	0.0043 (10)	−0.0027 (9)
C11	0.1026 (15)	0.0367 (11)	0.0379 (12)	−0.0006 (11)	0.0270 (12)	0.0049 (9)
C12	0.0733 (13)	0.0266 (9)	0.0777 (16)	0.0010 (9)	0.0538 (13)	0.0019 (11)
C13	0.0358 (10)	0.0399 (10)	0.0956 (18)	−0.0014 (8)	0.0192 (11)	0.0007 (11)
C14	0.0478 (10)	0.0373 (9)	0.0516 (13)	0.0035 (8)	0.0075 (10)	0.0085 (9)
C15	0.0431 (9)	0.0319 (9)	0.0359 (11)	−0.0035 (8)	0.0090 (8)	0.0034 (8)
C16	0.0362 (9)	0.0239 (8)	0.0330 (10)	0.0025 (7)	0.0083 (8)	0.0005 (8)
C17	0.0409 (9)	0.0441 (10)	0.0429 (12)	0.0172 (8)	0.0069 (9)	0.0032 (9)
C18	0.0499 (10)	0.0464 (10)	0.0380 (11)	0.0103 (8)	0.0054 (9)	−0.0061 (9)
C19	0.0425 (10)	0.0282 (8)	0.0507 (12)	0.0036 (7)	0.0181 (9)	−0.0056 (9)
C20	0.0324 (9)	0.0636 (12)	0.0584 (14)	0.0069 (8)	0.0060 (10)	−0.0090 (11)
C21	0.0392 (9)	0.0562 (10)	0.0433 (11)	0.0010 (8)	0.0030 (9)	−0.0110 (9)

Geometric parameters (Å, °)

Cl1—C19	1.7410 (14)	C8—H8A	0.9900
Cl2A—C12	1.793 (6)	C9—C10	1.3630 (19)
Cl2B—C12	1.7556 (17)	C9—C14	1.3722 (18)
O1—C1	1.2367 (14)	C10—C11	1.386 (2)
N1—C7	1.3815 (16)	C10—H10A	0.9400
N1—C8	1.4457 (17)	C11—C12	1.359 (2)
N1—H1A	0.854 (12)	C11—H11A	0.9400
N2—C1	1.3722 (16)	C12—C13	1.361 (2)
N2—N3	1.4258 (14)	C13—C14	1.384 (2)
N2—C8	1.4878 (15)	C13—H13A	0.9400
N3—C15	1.2610 (15)	C14—H14A	0.9400
C1—C2	1.4789 (17)	C15—C16	1.4677 (18)
C2—C3	1.3892 (17)	C15—H15A	0.9400
C2—C7	1.3929 (17)	C16—C21	1.3723 (17)
C3—C4	1.3786 (17)	C16—C17	1.3786 (18)
C3—H3A	0.9400	C17—C18	1.3814 (18)
C4—C5	1.3862 (18)	C17—H17A	0.9400
C4—H4A	0.9400	C18—C19	1.3724 (18)
C5—C6	1.3699 (17)	C18—H18A	0.9400
C5—H5A	0.9400	C19—C20	1.361 (2)
C6—C7	1.3924 (16)	C20—C21	1.3861 (19)
C6—H6A	0.9400	C20—H20A	0.9400
C8—C9	1.5090 (17)	C21—H21A	0.9400
C7—N1—C8	117.04 (12)	C9—C10—H10A	119.5
C7—N1—H1A	115.9 (9)	C11—C10—H10A	119.5
C8—N1—H1A	113.8 (9)	C12—C11—C10	118.91 (16)

C1—N2—N3	118.10 (10)	C12—C11—H11A	120.5
C1—N2—C8	120.02 (10)	C10—C11—H11A	120.5
N3—N2—C8	109.70 (11)	C11—C12—C13	121.48 (16)
C15—N3—N2	114.02 (13)	C11—C12—Cl2B	122.01 (18)
O1—C1—N2	121.67 (12)	C13—C12—Cl2B	116.50 (18)
O1—C1—C2	122.99 (13)	C11—C12—Cl2A	92.0 (3)
N2—C1—C2	115.33 (12)	C13—C12—Cl2A	146.5 (4)
C3—C2—C7	119.76 (12)	Cl2B—C12—Cl2A	30.1 (3)
C3—C2—C1	120.20 (12)	C12—C13—C14	118.95 (17)
C7—C2—C1	120.03 (13)	C12—C13—H13A	120.5
C4—C3—C2	120.50 (13)	C14—C13—H13A	120.5
C4—C3—H3A	119.7	C9—C14—C13	120.71 (16)
C2—C3—H3A	119.7	C9—C14—H14A	119.6
C3—C4—C5	119.29 (14)	C13—C14—H14A	119.6
C3—C4—H4A	120.4	N3—C15—C16	120.56 (14)
C5—C4—H4A	120.4	N3—C15—H15A	119.7
C6—C5—C4	120.99 (14)	C16—C15—H15A	119.7
C6—C5—H5A	119.5	C21—C16—C17	118.64 (14)
C4—C5—H5A	119.5	C21—C16—C15	119.34 (15)
C5—C6—C7	120.02 (13)	C17—C16—C15	121.99 (13)
C5—C6—H6A	120.0	C16—C17—C18	121.34 (14)
C7—C6—H6A	120.0	C16—C17—H17A	119.3
N1—C7—C6	122.02 (12)	C18—C17—H17A	119.3
N1—C7—C2	118.53 (12)	C19—C18—C17	118.64 (15)
C6—C7—C2	119.41 (13)	C19—C18—H18A	120.7
N1—C8—N2	106.24 (12)	C17—C18—H18A	120.7
N1—C8—C9	110.14 (11)	C20—C19—C18	121.11 (15)
N2—C8—C9	110.50 (10)	C20—C19—Cl1	119.17 (13)
N1—C8—H8A	110.0	C18—C19—Cl1	119.71 (14)
N2—C8—H8A	110.0	C19—C20—C21	119.64 (15)
C9—C8—H8A	110.0	C19—C20—H20A	120.2
C10—C9—C14	119.02 (14)	C21—C20—H20A	120.2
C10—C9—C8	121.07 (14)	C16—C21—C20	120.54 (16)
C14—C9—C8	119.92 (14)	C16—C21—H21A	119.7
C9—C10—C11	120.92 (16)	C20—C21—H21A	119.7
C1—N2—N3—C15	72.35 (15)	N1—C8—C9—C10	117.64 (15)
C8—N2—N3—C15	−145.13 (11)	N2—C8—C9—C10	−125.28 (14)
N3—N2—C1—O1	−20.85 (19)	N1—C8—C9—C14	−62.48 (16)
C8—N2—C1—O1	−159.42 (13)	N2—C8—C9—C14	54.59 (17)
N3—N2—C1—C2	159.47 (11)	C14—C9—C10—C11	−1.3 (2)
C8—N2—C1—C2	20.89 (18)	C8—C9—C10—C11	178.60 (13)
O1—C1—C2—C3	4.3 (2)	C9—C10—C11—C12	0.7 (2)
N2—C1—C2—C3	−176.04 (12)	C10—C11—C12—C13	0.3 (2)
O1—C1—C2—C7	−174.11 (13)	C10—C11—C12—Cl2B	−179.45 (11)
N2—C1—C2—C7	5.58 (19)	C10—C11—C12—Cl2A	179.9 (2)
C7—C2—C3—C4	−0.5 (2)	C11—C12—C13—C14	−0.7 (2)
C1—C2—C3—C4	−178.91 (13)	Cl2B—C12—C13—C14	179.05 (11)
C2—C3—C4—C5	1.7 (2)	Cl2A—C12—C13—C14	−180.0 (3)
C3—C4—C5—C6	−1.2 (2)	C10—C9—C14—C13	0.8 (2)

C4—C5—C6—C7	−0.3 (2)	C8—C9—C14—C13	−179.04 (12)
C8—N1—C7—C6	150.60 (13)	C12—C13—C14—C9	0.1 (2)
C8—N1—C7—C2	−31.76 (19)	N2—N3—C15—C16	−179.84 (11)
C5—C6—C7—N1	179.12 (13)	N3—C15—C16—C21	−165.09 (13)
C5—C6—C7—C2	1.5 (2)	N3—C15—C16—C17	13.2 (2)
C3—C2—C7—N1	−178.77 (13)	C21—C16—C17—C18	2.7 (2)
C1—C2—C7—N1	−0.4 (2)	C15—C16—C17—C18	−175.57 (13)
C3—C2—C7—C6	−1.1 (2)	C16—C17—C18—C19	−0.5 (2)
C1—C2—C7—C6	177.32 (13)	C17—C18—C19—C20	−1.9 (2)
C7—N1—C8—N2	53.23 (15)	C17—C18—C19—Cl1	179.14 (11)
C7—N1—C8—C9	172.93 (12)	C18—C19—C20—C21	2.0 (2)
C1—N2—C8—N1	−48.54 (15)	Cl1—C19—C20—C21	−179.03 (12)
N3—N2—C8—N1	169.77 (10)	C17—C16—C21—C20	−2.6 (2)
C1—N2—C8—C9	−168.00 (13)	C15—C16—C21—C20	175.72 (14)
N3—N2—C8—C9	50.31 (15)	C19—C20—C21—C16	0.3 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O1^{i}	0.854 (12)	2.153 (13)	2.9877 (15)	165.7 (12)

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

Fig. 1

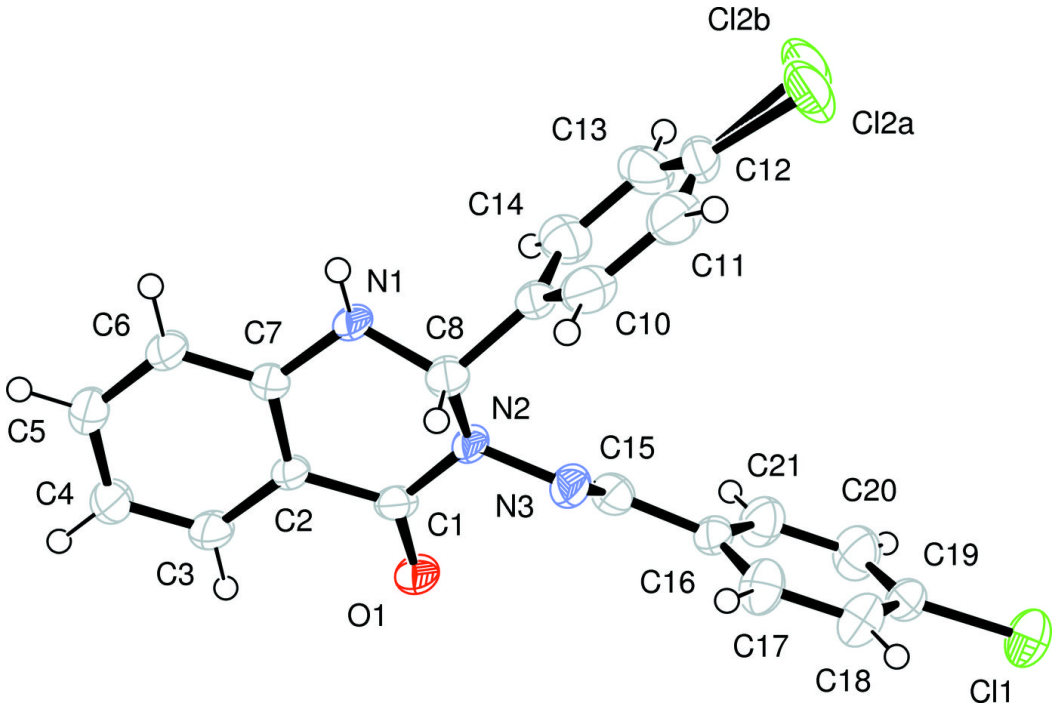
Cl2b
Cl2a
C13
C12
C14
C11
N1
C6
C7
C8
C10
C5
N2
C15
C21
C20
C4
C2
C1
N3
C19
C3
C16
O1
C17
C18
Cl1

Fig. 2