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2-{3-[2-(2-Chlorophenyl)ethyl]-2-oxo-1,2-dihydroquinoxalin-1-yl}acetohydrazide

Youssef Ramli,[a] Mohcine Missioui,[b,a]* Mohammed El Fal,[a] Mohammed Ouhcine,[b] El Mokhtar Essassi[c] and Joel T Mague[d]

[a]Laboratory of Medicinal Chemistry, Faculty of Medicine and Pharmacy, Mohammed V University, Rabat, Morocco, [b]Laboratory of Agrophysiology, Biotechnology, Environnement and Quality, Faculty of Science, Ibn Tofail University, Kenitra, Morocco, [c]Laboratoire de Chimie Organique Heterocyclique URAC 21, Av. Ibn Battouta, BP 1014, Faculte des Sciences, Universite Mohammed V, Rabat, Morocco, and [d]Department of Chemistry, Tulane University, New Orleans, LA 70118, USA. *Correspondence e-mail: mohcinemissioui@yahoo.com

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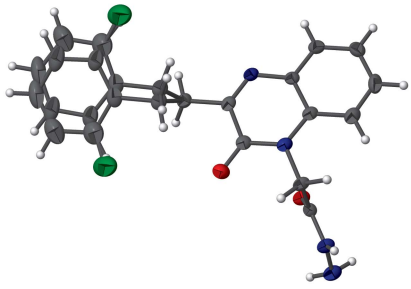
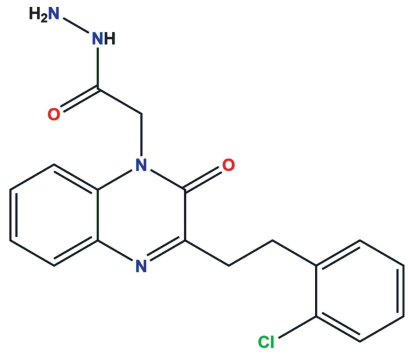
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{18}H_{17}ClN_4O_2$, the dihydroquinoxaline moiety deviates slightly from planarity. The benzene ring and its chloro and methylene substituents are disordered over two sets of sites, with an occupancy ratio of 0.675 (3):0.325 (3). In the crystal, corrugated sheets parallel to (100) are formed by N—H···O, N—H···Cl and N—H···N hydrogen bonds. The structure was refined as a two-component inversion twin.

3D view



Chemical scheme



Structure description

Among the various classes of nitrogen heterocyclic compounds, quinoxaline derivatives display a broad spectrum of biological activities (Ramli *et al.*, 2014). Some analogs have been synthesized and evaluated for their antimicrobial activity and many possess diverse biological activities including insecticidal, fungicidal, herbicidal, anthelmintic and antiviral (Ramli & Essassi, 2015). As a continuation of our work on the development of N-substituted quinoxaline-2-one derivatives in order to evaluate their pharmacological activity, we have studied the condensation reaction of ethyl 2-[3-(2-chlorophenethyl)-2-oxoquinoxalin-1(2*H*)-yl]acetate with hydrazine hydrate in ethanol to form the title compound (Fig. 1) in good yield (Ramli *et al.*, 2011, 2013; Caleb *et al.*, 2016).

The bicyclic core of the title compound is not quite planar, as indicated by the dihedral angle of 1.52 (16)° between the pyrazinone and the benzene rings. The pyrazinone ring is inclined to the major disorder component of the chlorophenyl ring by 24.80 (19)°. In the crystal, the molecules form zigzag chains running along the *c*-axis direction through N4—H4*A*···N2 hydrogen bonds together with weak N4—H4*B*···Cl1 interactions (Table 1 and

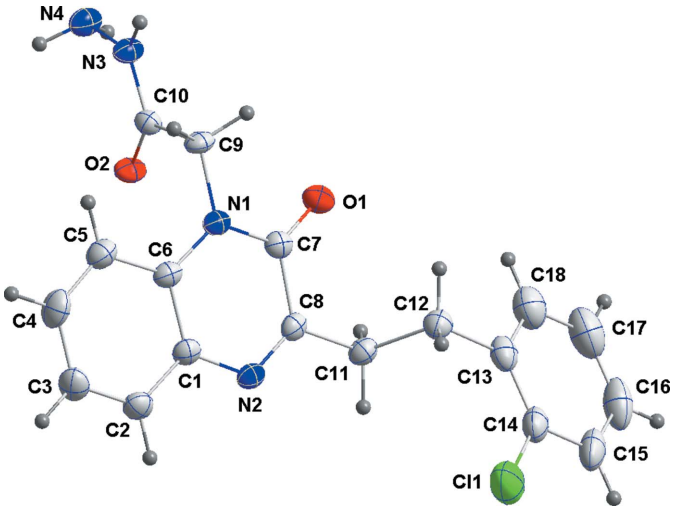


Figure 1
The title molecule with the labelling scheme and 50% probability displacement ellipsoids. Only the major disorder component is shown for clarity.

Fig. 2). N3—H3*A*···O2 hydrogen bonds form chains along *b* (Table 1 and Fig. 2) and combine with the sheets shown in Fig. 3 to form corrugated sheets parallel to (100).

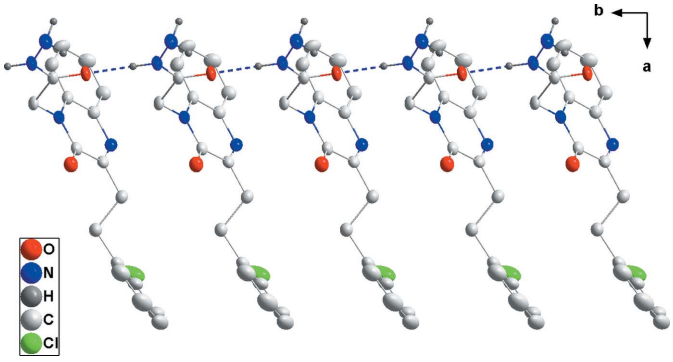


Figure 2
Chains of molecules formed along *b* by N—H···O hydrogen bonds.

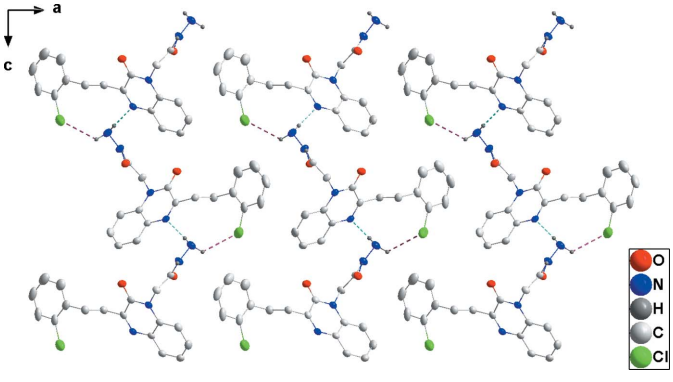


Figure 3
A view of the zigzag chains formed by N—H···N (light-blue dashed lines) and N—H···Cl (purple dashed lines) hydrogen bonds projected onto [010].

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···O2^{i}	0.91	1.96	2.842 (4)	163
N4—H4*A*···N2^{ii}	0.91	2.35	3.256 (4)	175
N4—H4*B*···Cl1^{ii}	0.91	2.92	3.539 (3)	126

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{17}ClN_4O_2$
M_r	356.80
Crystal system, space group	Orthorhombic, *Pna*2$_1$
Temperature (K)	100
a, *b*, *c* (Å)	24.258 (3), 4.6484 (5), 14.7708 (16)
V (Å^3)	1665.6 (3)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	0.25
Crystal size (mm)	0.25 × 0.16 × 0.05
Data collection	
Diffractometer	Bruker SMART APEX CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.94, 0.99
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7372, 4036, 3379
R_{int}	0.027
(sin θ/λ)$_{max}$ (Å^{-1})	0.668
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.052, 0.145, 1.07
No. of reflections	4036
No. of parameters	231
No. of restraints	84
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.77, −0.30
Absolute structure	Refined as an inversion twin
Absolute structure parameter	0.49 (16)

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

Synthesis and crystallization

To a solution of ethyl 2-[3-(2-chlorophenethyl)-2-oxoquinoxalin-1(2*H*)-yl]acetate (2.70 mmol, 1 g) in 20 ml of ethanol, hydrazine hydrate (4.58 mmol, 229.49 mg) was added. The mixture was stirred at room temperature for 24 h. The solid material was removed by filtration and the solvent evaporated under vacuum. The solid product was purified by recrystallization from ethanol solution to afford colorless block-like crystals of the title compound (yield 63%).

Refinement

Crystal and refinement details are presented in Table 2. The 2-chlorobenzyl group is disordered over several closely spaced positions. After several attempts, the only feasible model was a two-site one, treating the rings as rigid hexagons. The structure was refined as a two-component inversion twin.

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x171424 [https://doi.org/10.1107/S2414314617014249]

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2-{3-[2-(2-Chlorophenyl)ethyl]-2-oxo-1,2-dihydroquinoxalin-1-yl}acetohydrazide

Crystal data

$C_{18}H_{17}ClN_4O_2$
M_r = 356.80
Orthorhombic, $Pna2_1$
a = 24.258 (3) Å
b = 4.6484 (5) Å
c = 14.7708 (16) Å
V = 1665.6 (3) Å^3
Z = 4
$F(000)$ = 744
D_x = 1.423 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6865 reflections
θ = 2.2–27.5°
μ = 0.25 mm^{-1}
T = 100 K
Block, colorless
0.25 × 0.16 × 0.05 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.3333 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
T_{min} = 0.94, T_{max} = 0.99
7372 measured reflections
4036 independent reflections
3379 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 28.3°, θ_{min} = 1.7°
h = −32→32
k = −6→6
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.145
S = 1.07
4036 reflections
231 parameters
84 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0818P)^2 + 0.3986P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.77 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}
Absolute structure: Refined as an inversion twin
Absolute structure parameter: 0.49 (16)

Special details

Experimental. The diffraction data were collected in three sets of 363 frames (0.5° width in ω) at φ = 0, 120 and 240°. A scan time of 180 sec/frame was used.

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. The 2-chlorobenzyl group is disordered over several closely spaced positions. After several attempts, the only feasible model was a 2-site one treating the rings as rigid hexagons. H-atoms attached to carbon were placed in idealized positions while those attached to nitrogen were placed in locations derived from a difference map and their coordinates adjusted to give N—H = 0.91 %A. All were included as riding contributions. Refined as a 2-component inversion twin.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.57433 (10)	0.7964 (6)	0.42015 (17)	0.0305 (6)	
O2	0.43551 (10)	0.6782 (5)	0.38490 (17)	0.0267 (5)	
N1	0.50239 (11)	0.8913 (6)	0.51467 (18)	0.0231 (6)	
N2	0.54455 (12)	0.4766 (6)	0.63241 (19)	0.0242 (6)	
N3	0.41985 (12)	1.1092 (6)	0.3195 (2)	0.0263 (6)	
H3A	0.4245	1.3014	0.3283	0.034 (11)*	
N4	0.38670 (13)	0.9972 (7)	0.2490 (2)	0.0317 (7)	
H4A	0.4043	0.8569	0.2173	0.044 (13)*	
H4B	0.3559	0.9345	0.2781	0.038 (12)*	
C1	0.49487 (13)	0.6127 (7)	0.6508 (2)	0.0233 (6)	
C2	0.46541 (15)	0.5374 (8)	0.7293 (2)	0.0293 (7)	
H2	0.4799	0.3950	0.7688	0.035*	
C3	0.41607 (16)	0.6664 (9)	0.7498 (2)	0.0339 (8)	
H3	0.3969	0.6161	0.8036	0.041*	
C4	0.39449 (15)	0.8702 (9)	0.6914 (3)	0.0374 (9)	
H4	0.3602	0.9581	0.7056	0.045*	
C5	0.42163 (15)	0.9485 (8)	0.6132 (3)	0.0312 (8)	
H5	0.4059	1.0881	0.5740	0.037*	
C6	0.47239 (14)	0.8223 (7)	0.5917 (2)	0.0234 (7)	
C7	0.55016 (14)	0.7508 (7)	0.4917 (2)	0.0234 (6)	
C8	0.57052 (13)	0.5406 (7)	0.5594 (2)	0.0237 (7)	
C9	0.48067 (14)	1.0949 (7)	0.4481 (2)	0.0246 (7)	
H9A	0.5116	1.1848	0.4147	0.030*	
H9B	0.4600	1.2491	0.4795	0.030*	
C10	0.44243 (13)	0.9402 (7)	0.3812 (2)	0.0215 (6)	
C11	0.62385 (13)	0.3913 (7)	0.5368 (2)	0.0261 (7)	
H11A	0.6205	0.3004	0.4764	0.031*	
H11B	0.6305	0.2368	0.5816	0.031*	
Cl1	0.74190 (7)	0.3151 (6)	0.69305 (14)	0.0692 (6)	0.675 (3)
C12	0.6744 (3)	0.6004 (17)	0.5363 (5)	0.0297 (18)	0.675 (3)

H12A	0.6689	0.7525	0.4903	0.036*	0.675 (3)
H12B	0.6783	0.6934	0.5963	0.036*	0.675 (3)
C13	0.72605 (16)	0.4260 (10)	0.5144 (3)	0.0332 (14)	0.675 (3)
C14	0.75662 (17)	0.2843 (10)	0.5803 (3)	0.0384 (14)	0.675 (3)
C15	0.80138 (15)	0.1150 (10)	0.5555 (4)	0.0494 (16)	0.675 (3)
H15	0.8223	0.0182	0.6005	0.059*	0.675 (3)
C16	0.81556 (16)	0.0875 (11)	0.4647 (4)	0.054 (2)	0.675 (3)
H16	0.8462	−0.0281	0.4477	0.065*	0.675 (3)
C17	0.7850 (2)	0.2293 (13)	0.3988 (3)	0.061 (2)	0.675 (3)
H17	0.7947	0.2105	0.3367	0.073*	0.675 (3)
C18	0.7402 (2)	0.3985 (12)	0.4236 (3)	0.0528 (18)	0.675 (3)
H18	0.7193	0.4953	0.3786	0.063*	0.675 (3)
Cl1A	0.71901 (15)	0.5143 (12)	0.3615 (3)	0.0692 (6)	0.325 (3)
C12A	0.6753 (6)	0.566 (4)	0.5630 (14)	0.0297 (18)	0.325 (3)
H12C	0.6766	0.7474	0.5279	0.036*	0.325 (3)
H12D	0.6742	0.6146	0.6282	0.036*	0.325 (3)
C13A	0.7262 (4)	0.383 (2)	0.5423 (8)	0.0332 (14)	0.325 (3)
C14A	0.7474 (4)	0.345 (2)	0.4556 (7)	0.0384 (14)	0.325 (3)
C15A	0.7933 (4)	0.171 (2)	0.4423 (6)	0.0494 (16)	0.325 (3)
H15A	0.8077	0.1451	0.3830	0.059*	0.325 (3)
C16A	0.8180 (4)	0.035 (2)	0.5155 (8)	0.054 (2)	0.325 (3)
H16A	0.8494	−0.0840	0.5064	0.065*	0.325 (3)
C17A	0.7969 (4)	0.073 (3)	0.6022 (7)	0.061 (2)	0.325 (3)
H17A	0.8138	−0.0203	0.6523	0.073*	0.325 (3)
C18A	0.7510 (5)	0.247 (3)	0.6156 (6)	0.0528 (18)	0.325 (3)
H18A	0.7365	0.2725	0.6748	0.063*	0.325 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0359 (13)	0.0295 (13)	0.0259 (12)	−0.0008 (10)	0.0010 (10)	0.0006 (10)
O2	0.0348 (12)	0.0148 (10)	0.0304 (12)	−0.0028 (9)	−0.0054 (10)	0.0007 (9)
N1	0.0264 (13)	0.0183 (12)	0.0245 (13)	−0.0020 (11)	−0.0054 (11)	−0.0004 (11)
N2	0.0259 (13)	0.0234 (14)	0.0232 (13)	0.0003 (11)	−0.0059 (11)	−0.0006 (11)
N3	0.0324 (14)	0.0174 (13)	0.0292 (15)	−0.0031 (11)	−0.0085 (11)	0.0012 (11)
N4	0.0362 (16)	0.0261 (15)	0.0328 (16)	−0.0027 (13)	−0.0106 (13)	−0.0001 (12)
C1	0.0261 (15)	0.0233 (15)	0.0204 (14)	−0.0009 (12)	−0.0041 (12)	−0.0023 (12)
C2	0.0308 (18)	0.0328 (18)	0.0244 (16)	−0.0013 (14)	−0.0047 (13)	0.0016 (15)
C3	0.0319 (18)	0.045 (2)	0.0244 (17)	−0.0014 (16)	0.0015 (14)	−0.0027 (16)
C4	0.0275 (17)	0.043 (2)	0.042 (2)	0.0081 (16)	0.0027 (15)	−0.0094 (18)
C5	0.0309 (18)	0.0278 (19)	0.0349 (19)	0.0032 (14)	−0.0048 (14)	0.0001 (14)
C6	0.0278 (16)	0.0187 (15)	0.0237 (15)	−0.0005 (12)	−0.0061 (12)	−0.0018 (12)
C7	0.0272 (16)	0.0187 (15)	0.0243 (15)	−0.0028 (12)	−0.0031 (11)	−0.0032 (12)
C8	0.0227 (15)	0.0202 (15)	0.0281 (16)	−0.0022 (12)	−0.0061 (12)	−0.0025 (13)
C9	0.0303 (16)	0.0157 (15)	0.0278 (16)	0.0013 (13)	−0.0063 (12)	0.0034 (12)
C10	0.0248 (14)	0.0176 (15)	0.0221 (14)	−0.0005 (11)	0.0016 (12)	−0.0009 (12)
C11	0.0271 (15)	0.0237 (16)	0.0276 (16)	0.0028 (13)	−0.0033 (13)	−0.0019 (13)
Cl1	0.0429 (8)	0.1067 (17)	0.0581 (9)	−0.0183 (9)	−0.0076 (7)	0.0194 (11)

C12	0.0289 (18)	0.025 (3)	0.036 (5)	0.0000 (18)	−0.001 (3)	0.000 (3)
C13	0.0282 (18)	0.026 (2)	0.045 (4)	−0.0052 (17)	0.005 (2)	−0.004 (3)
C14	0.023 (2)	0.035 (3)	0.057 (4)	−0.004 (2)	0.001 (2)	0.003 (3)
C15	0.023 (2)	0.040 (3)	0.085 (4)	−0.003 (2)	0.000 (3)	0.002 (3)
C16	0.033 (2)	0.043 (3)	0.086 (6)	−0.004 (2)	0.017 (4)	−0.023 (4)
C17	0.051 (3)	0.062 (4)	0.068 (4)	−0.015 (3)	0.019 (3)	−0.014 (3)
C18	0.043 (3)	0.053 (4)	0.062 (4)	−0.011 (3)	0.005 (3)	−0.001 (3)
Cl1A	0.0429 (8)	0.1067 (17)	0.0581 (9)	−0.0183 (9)	−0.0076 (7)	0.0194 (11)
C12A	0.0289 (18)	0.025 (3)	0.036 (5)	0.0000 (18)	−0.001 (3)	0.000 (3)
C13A	0.0282 (18)	0.026 (2)	0.045 (4)	−0.0052 (17)	0.005 (2)	−0.004 (3)
C14A	0.023 (2)	0.035 (3)	0.057 (4)	−0.004 (2)	0.001 (2)	0.003 (3)
C15A	0.023 (2)	0.040 (3)	0.085 (4)	−0.003 (2)	0.000 (3)	0.002 (3)
C16A	0.033 (2)	0.043 (3)	0.086 (6)	−0.004 (2)	0.017 (4)	−0.023 (4)
C17A	0.051 (3)	0.062 (4)	0.068 (4)	−0.015 (3)	0.019 (3)	−0.014 (3)
C18A	0.043 (3)	0.053 (4)	0.062 (4)	−0.011 (3)	0.005 (3)	−0.001 (3)

Geometric parameters (Å, º)

O1—C7	1.227 (4)	C11—H11B	0.9900
O2—C10	1.231 (4)	Cl1—C14	1.709 (4)
N1—C7	1.373 (4)	C12—C13	1.528 (8)
N1—C6	1.389 (4)	C12—H12A	0.9900
N1—C9	1.463 (4)	C12—H12B	0.9900
N2—C8	1.284 (5)	C13—C14	1.3900
N2—C1	1.388 (4)	C13—C18	1.3900
N3—C10	1.323 (4)	C14—C15	1.3900
N3—N4	1.414 (4)	C15—C16	1.3900
N3—H3A	0.9099	C15—H15	0.9500
N4—H4A	0.9100	C16—C17	1.3900
N4—H4B	0.9100	C16—H16	0.9500
C1—C2	1.407 (5)	C17—C18	1.3900
C1—C6	1.416 (4)	C17—H17	0.9500
C2—C3	1.372 (5)	C18—H18	0.9500
C2—H2	0.9500	Cl1A—C14A	1.740 (9)
C3—C4	1.384 (6)	C12A—C13A	1.533 (18)
C3—H3	0.9500	C12A—H12C	0.9900
C4—C5	1.378 (6)	C12A—H12D	0.9900
C4—H4	0.9500	C13A—C14A	1.3900
C5—C6	1.401 (5)	C13A—C18A	1.3900
C5—H5	0.9500	C14A—C15A	1.3900
C7—C8	1.483 (5)	C15A—C16A	1.3900
C8—C11	1.506 (4)	C15A—H15A	0.9500
C9—C10	1.533 (4)	C16A—C17A	1.3900
C9—H9A	0.9900	C16A—H16A	0.9500
C9—H9B	0.9900	C17A—C18A	1.3900
C11—C12A	1.538 (16)	C17A—H17A	0.9500
C11—C12	1.564 (8)	C18A—H18A	0.9500
C11—H11A	0.9900		

C7—N1—C6	122.4 (3)	H11A—C11—H11B	107.8
C7—N1—C9	116.4 (3)	C13—C12—C11	108.3 (5)
C6—N1—C9	120.8 (3)	C13—C12—H12A	110.0
C8—N2—C1	119.0 (3)	C11—C12—H12A	110.0
C10—N3—N4	121.6 (3)	C13—C12—H12B	110.0
C10—N3—H3A	115.7	C11—C12—H12B	110.0
N4—N3—H3A	122.5	H12A—C12—H12B	108.4
N3—N4—H4A	112.1	C14—C13—C18	120.0
N3—N4—H4B	103.7	C14—C13—C12	122.7 (4)
H4A—N4—H4B	113.5	C18—C13—C12	117.2 (4)
N2—C1—C2	119.2 (3)	C15—C14—C13	120.0
N2—C1—C6	121.8 (3)	C15—C14—Cl1	117.9 (3)
C2—C1—C6	118.9 (3)	C13—C14—Cl1	122.1 (3)
C3—C2—C1	121.0 (3)	C14—C15—C16	120.0
C3—C2—H2	119.5	C14—C15—H15	120.0
C1—C2—H2	119.5	C16—C15—H15	120.0
C2—C3—C4	119.5 (3)	C17—C16—C15	120.0
C2—C3—H3	120.3	C17—C16—H16	120.0
C4—C3—H3	120.3	C15—C16—H16	120.0
C5—C4—C3	121.5 (3)	C16—C17—C18	120.0
C5—C4—H4	119.3	C16—C17—H17	120.0
C3—C4—H4	119.3	C18—C17—H17	120.0
C4—C5—C6	120.0 (3)	C17—C18—C13	120.0
C4—C5—H5	120.0	C17—C18—H18	120.0
C6—C5—H5	120.0	C13—C18—H18	120.0
N1—C6—C5	123.4 (3)	C13A—C12A—C11	108.1 (11)
N1—C6—C1	117.5 (3)	C13A—C12A—H12C	110.1
C5—C6—C1	119.1 (3)	C11—C12A—H12C	110.1
O1—C7—N1	122.3 (3)	C13A—C12A—H12D	110.1
O1—C7—C8	122.4 (3)	C11—C12A—H12D	110.1
N1—C7—C8	115.3 (3)	H12C—C12A—H12D	108.4
N2—C8—C7	123.8 (3)	C14A—C13A—C18A	120.0
N2—C8—C11	120.1 (3)	C14A—C13A—C12A	123.5 (10)
C7—C8—C11	116.1 (3)	C18A—C13A—C12A	116.5 (10)
N1—C9—C10	110.3 (3)	C15A—C14A—C13A	120.0
N1—C9—H9A	109.6	C15A—C14A—Cl1A	117.8 (6)
C10—C9—H9A	109.6	C13A—C14A—Cl1A	122.2 (6)
N1—C9—H9B	109.6	C14A—C15A—C16A	120.0
C10—C9—H9B	109.6	C14A—C15A—H15A	120.0
H9A—C9—H9B	108.1	C16A—C15A—H15A	120.0
O2—C10—N3	124.2 (3)	C15A—C16A—C17A	120.0
O2—C10—C9	121.2 (3)	C15A—C16A—H16A	120.0
N3—C10—C9	114.6 (3)	C17A—C16A—H16A	120.0
C8—C11—C12A	113.4 (8)	C18A—C17A—C16A	120.0
C8—C11—C12	112.8 (4)	C18A—C17A—H17A	120.0
C8—C11—H11A	109.0	C16A—C17A—H17A	120.0
C12—C11—H11A	109.0	C17A—C18A—C13A	120.0

C8—C11—H11B	109.0	C17A—C18A—H18A	120.0
C12—C11—H11B	109.0	C13A—C18A—H18A	120.0
C8—N2—C1—C2	178.2 (3)	N2—C8—C11—C12A	−97.9 (9)
C8—N2—C1—C6	−0.7 (5)	C7—C8—C11—C12A	84.3 (9)
N2—C1—C2—C3	−179.8 (3)	N2—C8—C11—C12	−115.1 (4)
C6—C1—C2—C3	−0.9 (5)	C7—C8—C11—C12	67.1 (4)
C1—C2—C3—C4	1.1 (6)	C8—C11—C12—C13	179.0 (4)
C2—C3—C4—C5	−0.4 (6)	C11—C12—C13—C14	−86.4 (5)
C3—C4—C5—C6	−0.4 (6)	C11—C12—C13—C18	89.8 (4)
C7—N1—C6—C5	−175.4 (3)	C18—C13—C14—C15	0.0
C9—N1—C6—C5	−3.0 (5)	C12—C13—C14—C15	176.2 (5)
C7—N1—C6—C1	4.5 (4)	C18—C13—C14—Cl1	178.8 (4)
C9—N1—C6—C1	176.9 (3)	C12—C13—C14—Cl1	−5.0 (5)
C4—C5—C6—N1	−179.5 (3)	C13—C14—C15—C16	0.0
C4—C5—C6—C1	0.6 (5)	Cl1—C14—C15—C16	−178.9 (4)
N2—C1—C6—N1	−1.0 (5)	C14—C15—C16—C17	0.0
C2—C1—C6—N1	−179.8 (3)	C15—C16—C17—C18	0.0
N2—C1—C6—C5	178.9 (3)	C16—C17—C18—C13	0.0
C2—C1—C6—C5	0.1 (5)	C14—C13—C18—C17	0.0
C6—N1—C7—O1	174.3 (3)	C12—C13—C18—C17	−176.4 (4)
C9—N1—C7—O1	1.6 (5)	C8—C11—C12A—C13A	176.3 (8)
C6—N1—C7—C8	−5.9 (4)	C11—C12A—C13A—C14A	77.5 (13)
C9—N1—C7—C8	−178.6 (3)	C11—C12A—C13A—C18A	−101.4 (12)
C1—N2—C8—C7	−1.0 (5)	C18A—C13A—C14A—C15A	0.0
C1—N2—C8—C11	−178.6 (3)	C12A—C13A—C14A—C15A	−178.9 (9)
O1—C7—C8—N2	−176.0 (3)	C18A—C13A—C14A—Cl1A	−178.8 (9)
N1—C7—C8—N2	4.2 (5)	C12A—C13A—C14A—Cl1A	2.3 (11)
O1—C7—C8—C11	1.8 (4)	C13A—C14A—C15A—C16A	0.0
N1—C7—C8—C11	−178.1 (3)	Cl1A—C14A—C15A—C16A	178.9 (8)
C7—N1—C9—C10	88.2 (3)	C14A—C15A—C16A—C17A	0.0
C6—N1—C9—C10	−84.6 (3)	C15A—C16A—C17A—C18A	0.0
N4—N3—C10—O2	−2.4 (5)	C16A—C17A—C18A—C13A	0.0
N4—N3—C10—C9	175.5 (3)	C14A—C13A—C18A—C17A	0.0
N1—C9—C10—O2	−3.5 (4)	C12A—C13A—C18A—C17A	179.0 (8)
N1—C9—C10—N3	178.6 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···O2^{i}	0.91	1.96	2.842 (4)	163
N4—H4*A*···N2^{ii}	0.91	2.35	3.256 (4)	175
N4—H4*B*···Cl1^{ii}	0.91	2.92	3.539 (3)	126

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