Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-(2,6-Dichlorophenyl)-*N*-(1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1*H*-pyrazol-4-yl)acetamide

Ray J. Butcher,[a]* Aneeka Mahan,[b] P. S. Nayak,[c] B. Narayana[c] and H. S. Yathirajan[d]

[a]Department of Chemistry, Howard University, 525 College Street NW, Washington, DC 20059, USA, [b]Lake Braddock Secondary School, 9200 Burke Lake Road, Burke, VA 22015, USA, [c]Department of Studies in Chemistry, Mangalore University, Mangalagangotri 574 199, India, and [d]Department of Studies in Chemistry, University of Mysore, Manasagangotri, Mysore 570 006, India
Correspondence e-mail: rbutcher99@yahoo.com

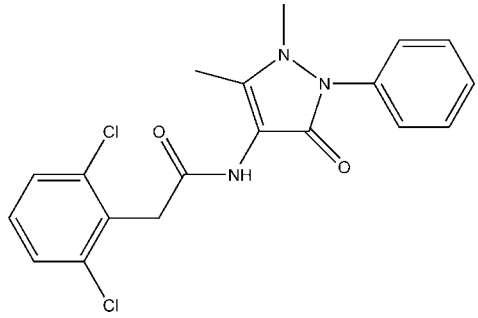
Received 2 December 2012; accepted 3 December 2012

Key indicators: single-crystal X-ray study; T = 123 K; mean σ(C–C) = 0.004 Å; R factor = 0.062; wR factor = 0.185; data-to-parameter ratio = 15.6.

In the title compound, $C_{19}H_{17}Cl_2N_3O_2$, the amide group is planar and, through N—H···O hydrogen bonding to an adjoining molecule, forms dimers of the $R_2^2(10)$ type. As a result of steric repulsion, the amide group is rotated with respect to both the dichlorophenyl and 2,3-dihydro-1*H*-pyrazol-4-yl rings, making dihedral angles of 71.63 (11) and 57.93 (10)°, respectively. The dihedral angle between the dichlorophenyl and 2,3-dihydro-1*H*-pyrazol-4-yl rings is 76.60 (10)° while that between the 2,3-dihydro-1*H*-pyrazol-4-yl and phenyl rings is 49.29 (7)°. The crystal structure also features weak C—H···O interactions.

Related literature

N-Substituted 2-arylacetamides are of interest because of their structural similarity to the lateral chain of natural benzylpenicillin, see: Mijin & Marinkovic (2006); Mijin *et al.* (2008). For amides as ligands, see: Wu *et al.* (2008, 2010). For the structures of acetamide derivatives, see: Fun *et al.* (2011*a*,*b*, 2012*a*,*b*). For a description of the Cambridge Structural Database, see: Allen (2002). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{19}H_{17}Cl_2N_3O_2$
M_r = 390.26
Monoclinic, $C2/c$
a = 20.3442 (11) Å
b = 12.1080 (8) Å
c = 14.9500 (8) Å
β = 93.837 (5)°
V = 3674.3 (4) Å^3
Z = 8
Cu $K\alpha$ radiation
μ = 3.34 mm^{-1}
T = 123 K
0.60 × 0.55 × 0.24 mm

Data collection

Agilent Xcalibur (Ruby, Gemini) diffractometer
Absorption correction: analytical [*CrysAlis PRO* (Agilent, 2011) based on expressions derived by Clark & Reid (1995)]
T_{min} = 0.276, T_{max} = 0.560
6894 measured reflections
3692 independent reflections
2836 reflections with $I > 2\sigma(I)$
R_{int} = 0.065

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.185
S = 1.05
3692 reflections
237 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.62 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*A*···O2^{i}	0.88	1.99	2.845 (3)	164
C7—H7*A*···O2^{i}	0.99	2.47	3.249 (3)	135
C12—H12*A*···O1^{ii}	0.98	2.43	3.104 (3)	126

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

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO* (Agilent, 2011); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

BN thanks the UGC for financial assistance through a BSR one-time grant for the purchase of chemicals. PSN thanks Mangalore University for research facilities and the DST–PURSE financial assistance. RJB acknowledges the NSF–MRI program (grant No. CHE-0619278) for funds to purchase the diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG5277).

References

Agilent. (2011). *CrysAlis PRO* and *CrysAlis RED*. Agilent Technologies, Yarnton, England.

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.

Clark, R. C. & Reid, J. S. (1995). *Acta Cryst.* A**51**, 887–897.

Fun, H.-K., Quah, C. K., Narayana, B., Nayak, P. S. & Sarojini, B. K. (2011*a*). *Acta Cryst.* E**67**, o2926–o2927.

Fun, H.-K., Quah, C. K., Narayana, B., Nayak, P. S. & Sarojini, B. K. (2011*b*). *Acta Cryst.* E**67**, o2941–o2942.

Fun, H.-K., Quah, C. K., Nayak, P. S., Narayana, B. & Sarojini, B. K. (2012*a*). *Acta Cryst.* E**68**, o2677.

Fun, H.-K., Shahani, T., Nayak, P. S., Narayana, B. & Sarojini, B. K. (2012*b*). *Acta Cryst.* E**68**, o519.

Mijin, D. & Marinkovic, A. (2006). *Synth. Commun.* **36**, 193–198.

Mijin, D. Z., Prascevic, M. & Petrovic, S. D. (2008). *J. Serb. Chem. Soc.* **73**, 945–950.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Wu, W.-N., Cheng, F.-X., Yan, L. & Tang, N. (2008). *J. Coord. Chem.* **61**, 2207–2215.

Wu, W.-N., Wang, Y., Zhang, A.-Y., Zhao, R.-Q. & Wang, Q.-F. (2010). *Acta Cryst.* E**66**, m288.

supplementary materials

Acta Cryst. (2013). E**69**, o46–o47 [doi:10.1107/S160053681204963X]

2-(2,6-Dichlorophenyl)-*N*-(1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1*H*-pyrazol-4-yl)acetamide

Ray J. Butcher, Aneeka Mahan, P. S. Nayak, B. Narayana and H. S. Yathirajan

Comment

N-Substituted 2-arylacetamides are very interesting compounds because of their structural similarity to the lateral chain of natural benzylpenicillin (Mijin *et al.*, 2006, 2008). Amides are also used as ligands due to their excellent coordination abilities (Wu *et al.*, 2008, 2010). Crystal structures of some acetamide derivatives *viz*., (2E)-1-(2,5-dimethoxyphenyl)-3-(3-nitrophenyl)prop-2-en-1-one, *N*-(4-bromophenyl)-2-(naphthalen-1-yl)acetamide, *N*-(1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1*H*-pyrazol-4-yl)-2-[4-(methylsulfanyl)phenyl]acetamide, *N*-(4-Bromophenyl)-2-(4-chlorophenyl)-acetamide (Fun *et al.*, 2011*a,b*, 2012*a*,*b*) have been reported. In view of the importance of amides we report herein the crystal structure of the title compound (I).

In the title compound, I, $C_{19}H_{17}Cl_2N_3O_2$ the amide group is planar and through N—H···O hydrogen bonding to an adjoining molecule forms dimers of the $R_2^2(10)$ type (Bernstein *et al.*, 1995). Due to steric repulsion the amide group is rotated with respect to both the dichlorophenyl and 2,3-dihydro-1*H*-pyrazol-4-yl rings with dihedral angles of 71.63 (11)° and 57.93 (10)° respectively. The dihedral angles between the three rings are 76.60 (10)° for the dichlorophenyl and 2,3-dihydro-1*H*-pyrazol-4-yl rings and and 49.29 (7)° for the 2,3-dihydro-1*H*-pyrazol-4-yl and phenyl rings, respectively. In addition there are weak intermolecular C—H···O interactions. All other metrical prameters are in the normal ranges (Allen, 2002).

Experimental

2,6-Dichlorophenylacetic acid (0.240 g, 1 mmol), 4-aminoantipyrine (0.203 g, 1 mmol) and 1-ethyl-3-(3-dimethylaminopropyl)-carbodiimide hydrochloride (1.0 g, 0.01 mol) were dissolved in dichloromethane (20 ml). The mixture was stirred in presence of triethylamine at 273 K for about 3 h. The contents were poured into 100 ml of ice-cold aqueous hydrochloric acid with stirring, which was extracted thrice with dichloromethane. Organic layer was washed with saturated $NaHCO_3$ solution and brine solution, dried and concentrated under reduced pressure to give the title compound (I). Single crystals were grown from methanol and acetone mixture (1:1) by the slow evaporation method (m.p.: 501–503 K).

Refinement

The H atoms were placed in calculated positions and refined in the riding mode: N—H = 0.88 Å, C—H = 0.95–0.99 Å with U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and = 1.2U_{eq}(O,*C*) for other H atoms.

Computing details

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO* (Agilent, 2011); data reduction: *CrysAlis PRO* (Agilent, 2011); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine

structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

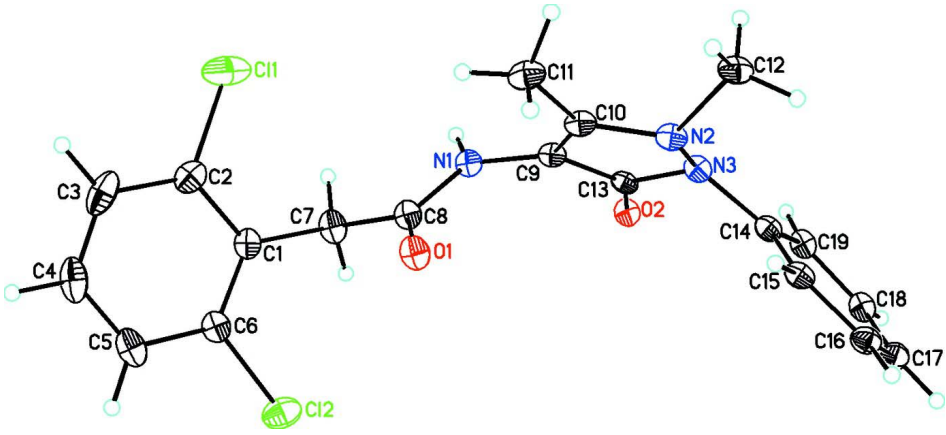


Figure 1

The molecular structure of the title molecule with the atom numbering. The displacement ellipsoids are drawn at the 30% probability level.

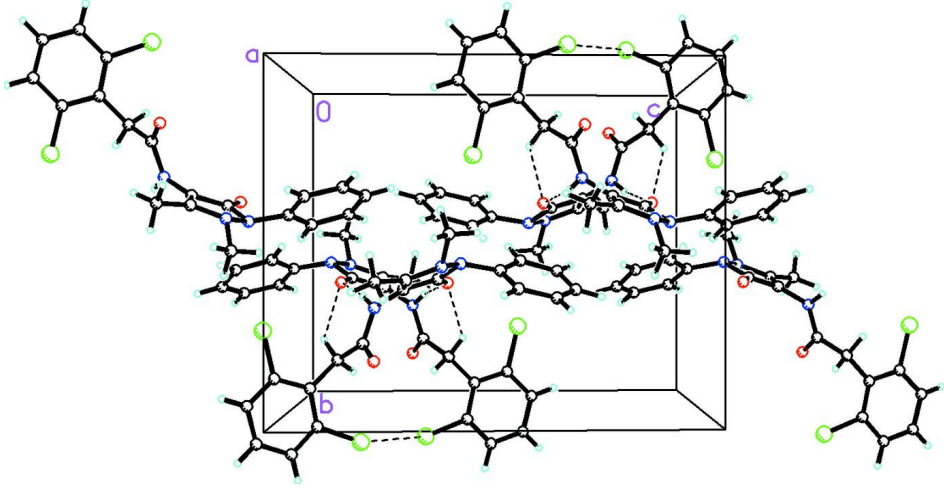


Figure 2

The crystal packing of the title compound, viewed along the *a* axis. Hydrogen bonds are shown as dashed lines - see Table 1 for details.

2-(2,6-Dichlorophenyl)-*N*-(1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro- 1*H*-pyrazol-4-yl)acetamide

Crystal data

$C_{19}H_{17}Cl_2N_3O_2$
$M_r = 390.26$
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
$a = 20.3442\ (11)$ Å
$b = 12.1080\ (8)$ Å
$c = 14.9500\ (8)$ Å
$\beta = 93.837\ (5)°$
$V = 3674.3\ (4)$ Å^3
$Z = 8$
$F(000) = 1616$
$D_x = 1.411$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 2393 reflections
$\theta = 3.0–75.9°$
$\mu = 3.34$ mm^{-1}
$T = 123$ K
Prism, colorless
0.60 × 0.55 × 0.24 mm

Data collection

Agilent Xcalibur (Ruby, Gemini) diffractometer
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 10.5081 pixels mm^{-1}
ω scans
Absorption correction: analytical [*CrysAlis PRO* (Agilent, 2011) based on expressions derived by Clark & Reid (1995)]
T_{min} = 0.276, T_{max} = 0.560
6894 measured reflections
3692 independent reflections
2836 reflections with $I > 2\sigma(I)$
R_{int} = 0.065
θ_{max} = 76.1°, θ_{min} = 4.3°
h = −25→17
k = −14→13
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.185
S = 1.05
3692 reflections
237 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
$w = 1/[\sigma^2(F_o^2) + (0.0919P)^2 + 2.7039P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.62 e Å^{-3}

Special details

Experimental. CrysAlisPro (Agilent Technologies, 2011) Analytical numeric absorption correction using a multifaceted crystal model based on expressions derived by R.C. Clark & J.S. Reid. (Clark, R. C. & Reid, J. S. (1995). Acta Cryst. A51, 887-897)

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 $F^2 > \sigma(F^2)$ 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Cl1	0.60120 (7)	0.75806 (10)	−0.05511 (9)	0.0942 (4)
Cl2	0.55602 (5)	1.09130 (9)	0.17378 (6)	0.0674 (3)
O1	0.65197 (10)	0.84440 (18)	0.21156 (15)	0.0483 (5)
O2	0.53366 (8)	0.62011 (15)	0.38199 (13)	0.0384 (4)
N1	0.58629 (10)	0.69208 (19)	0.20824 (15)	0.0368 (5)
H1A	0.5532	0.6580	0.1791	0.044*
N2	0.70088 (10)	0.56877 (19)	0.37326 (16)	0.0389 (5)
N3	0.64116 (10)	0.56119 (18)	0.41658 (15)	0.0361 (5)
C1	0.57761 (12)	0.9297 (2)	0.05381 (19)	0.0401 (6)
C2	0.59995 (15)	0.8983 (3)	−0.0287 (2)	0.0517 (7)
C3	0.62067 (15)	0.9765 (4)	−0.0903 (2)	0.0673 (11)
H3A	0.6348	0.9533	−0.1466	0.081*
C4	0.62042 (16)	1.0866 (4)	−0.0685 (3)	0.0630 (10)
H4A	0.6343	1.1397	−0.1100	0.076*

C5	0.60035 (15)	1.1204 (3)	0.0123 (3)	0.0560 (8)
H5A	0.6005	1.1965	0.0276	0.067*
C6	0.57985 (13)	1.0419 (2)	0.0715 (2)	0.0432 (6)
C7	0.55062 (14)	0.8480 (3)	0.1174 (2)	0.0485 (7)
H7A	0.5277	0.7886	0.0820	0.058*
H7B	0.5175	0.8856	0.1522	0.058*
C8	0.60213 (12)	0.7957 (2)	0.18258 (18)	0.0396 (6)
C9	0.62085 (12)	0.6371 (2)	0.27977 (17)	0.0345 (5)
C10	0.68553 (13)	0.6078 (2)	0.28850 (19)	0.0386 (5)
C11	0.73533 (15)	0.6115 (3)	0.2201 (2)	0.0500 (7)
H11A	0.7150	0.6413	0.1639	0.075*
H11B	0.7516	0.5367	0.2098	0.075*
H11C	0.7721	0.6589	0.2415	0.075*
C12	0.74646 (13)	0.4761 (3)	0.3919 (2)	0.0474 (7)
H12A	0.7865	0.4876	0.3600	0.071*
H12B	0.7252	0.4071	0.3716	0.071*
H12C	0.7581	0.4720	0.4565	0.071*
C13	0.59091 (12)	0.60777 (19)	0.36049 (17)	0.0328 (5)
C14	0.64444 (13)	0.5810 (2)	0.51087 (18)	0.0366 (5)
C15	0.69919 (13)	0.6324 (2)	0.55341 (19)	0.0392 (6)
H15A	0.7364	0.6495	0.5209	0.047*
C16	0.69888 (14)	0.6585 (2)	0.6438 (2)	0.0447 (6)
H16A	0.7366	0.6917	0.6736	0.054*
C17	0.64403 (15)	0.6366 (2)	0.6907 (2)	0.0466 (6)
H17A	0.6433	0.6576	0.7519	0.056*
C18	0.58991 (14)	0.5837 (2)	0.6480 (2)	0.0441 (6)
H18A	0.5522	0.5688	0.6802	0.053*
C19	0.59051 (13)	0.5527 (2)	0.55887 (19)	0.0406 (6)
H19A	0.5546	0.5127	0.5308	0.049*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0878 (8)	0.0868 (7)	0.1062 (9)	0.0214 (6)	−0.0073 (7)	−0.0455 (7)
Cl2	0.0517 (5)	0.0811 (6)	0.0699 (5)	0.0068 (4)	0.0073 (4)	−0.0209 (4)
O1	0.0335 (10)	0.0511 (11)	0.0600 (12)	−0.0147 (8)	0.0014 (9)	0.0098 (9)
O2	0.0220 (8)	0.0463 (10)	0.0477 (10)	0.0035 (7)	0.0085 (7)	0.0055 (8)
N1	0.0264 (10)	0.0412 (11)	0.0431 (11)	−0.0065 (8)	0.0058 (8)	0.0012 (9)
N2	0.0223 (10)	0.0439 (11)	0.0515 (12)	0.0034 (8)	0.0097 (9)	−0.0044 (9)
N3	0.0215 (9)	0.0405 (11)	0.0472 (12)	0.0016 (8)	0.0083 (8)	0.0018 (9)
C1	0.0233 (11)	0.0518 (15)	0.0453 (14)	−0.0026 (10)	0.0036 (10)	0.0061 (11)
C2	0.0337 (14)	0.071 (2)	0.0501 (16)	0.0045 (13)	0.0039 (12)	−0.0048 (14)
C3	0.0317 (14)	0.130 (4)	0.0406 (15)	0.0040 (18)	0.0074 (11)	0.0080 (19)
C4	0.0306 (14)	0.088 (3)	0.070 (2)	−0.0103 (15)	0.0014 (14)	0.0365 (19)
C5	0.0331 (14)	0.0568 (17)	0.077 (2)	−0.0092 (12)	−0.0039 (14)	0.0207 (15)
C6	0.0254 (11)	0.0506 (15)	0.0537 (15)	−0.0020 (11)	0.0039 (10)	0.0050 (12)
C7	0.0298 (13)	0.0562 (16)	0.0595 (17)	−0.0094 (12)	0.0033 (12)	0.0137 (13)
C8	0.0280 (12)	0.0448 (13)	0.0467 (14)	−0.0078 (10)	0.0085 (10)	0.0042 (11)
C9	0.0266 (11)	0.0348 (11)	0.0430 (12)	−0.0039 (9)	0.0082 (9)	−0.0037 (9)
C10	0.0282 (12)	0.0409 (12)	0.0475 (14)	−0.0041 (10)	0.0100 (10)	−0.0082 (10)

C11	0.0355 (14)	0.0576 (16)	0.0593 (17)	−0.0042 (12)	0.0209 (13)	−0.0130 (13)
C12	0.0279 (12)	0.0502 (15)	0.0635 (17)	0.0105 (11)	−0.0004 (11)	−0.0120 (13)
C13	0.0252 (11)	0.0279 (10)	0.0461 (13)	0.0019 (8)	0.0065 (9)	−0.0012 (9)
C14	0.0294 (12)	0.0336 (11)	0.0473 (14)	0.0026 (9)	0.0060 (10)	0.0025 (10)
C15	0.0302 (12)	0.0343 (12)	0.0537 (15)	0.0016 (9)	0.0073 (11)	0.0012 (10)
C16	0.0391 (14)	0.0386 (13)	0.0559 (16)	−0.0003 (11)	−0.0005 (12)	−0.0042 (11)
C17	0.0465 (16)	0.0466 (14)	0.0469 (14)	0.0079 (12)	0.0047 (12)	−0.0010 (12)
C18	0.0369 (14)	0.0475 (14)	0.0490 (15)	0.0046 (11)	0.0101 (11)	0.0093 (11)
C19	0.0281 (12)	0.0433 (13)	0.0506 (14)	−0.0003 (10)	0.0052 (10)	0.0074 (11)

Geometric parameters (Å, º)

Cl1—C2	1.744 (4)	C7—H7A	0.9900
Cl2—C6	1.741 (3)	C7—H7B	0.9900
O1—C8	1.227 (3)	C9—C10	1.361 (4)
O2—C13	1.238 (3)	C9—C13	1.433 (3)
N1—C8	1.357 (4)	C10—C11	1.487 (4)
N1—C9	1.407 (3)	C11—H11A	0.9800
N1—H1A	0.8800	C11—H11B	0.9800
N2—C10	1.369 (4)	C11—H11C	0.9800
N2—N3	1.417 (3)	C12—H12A	0.9800
N2—C12	1.470 (3)	C12—H12B	0.9800
N3—C13	1.397 (3)	C12—H12C	0.9800
N3—C14	1.427 (4)	C14—C15	1.392 (4)
C1—C6	1.384 (4)	C14—C19	1.393 (4)
C1—C2	1.395 (4)	C15—C16	1.387 (4)
C1—C7	1.502 (4)	C15—H15A	0.9500
C2—C3	1.405 (5)	C16—C17	1.383 (4)
C3—C4	1.373 (6)	C16—H16A	0.9500
C3—H3A	0.9500	C17—C18	1.391 (4)
C4—C5	1.363 (6)	C17—H17A	0.9500
C4—H4A	0.9500	C18—C19	1.385 (4)
C5—C6	1.381 (4)	C18—H18A	0.9500
C5—H5A	0.9500	C19—H19A	0.9500
C7—C8	1.520 (4)		

C8—N1—C9	122.4 (2)	N1—C9—C13	122.6 (2)
C8—N1—H1A	118.8	C9—C10—N2	109.7 (2)
C9—N1—H1A	118.8	C9—C10—C11	128.7 (3)
C10—N2—N3	107.2 (2)	N2—C10—C11	121.5 (3)
C10—N2—C12	122.8 (2)	C10—C11—H11A	109.5
N3—N2—C12	114.4 (2)	C10—C11—H11B	109.5
C13—N3—N2	108.4 (2)	H11A—C11—H11B	109.5
C13—N3—C14	120.6 (2)	C10—C11—H11C	109.5
N2—N3—C14	117.1 (2)	H11A—C11—H11C	109.5
C6—C1—C2	115.4 (3)	H11B—C11—H11C	109.5
C6—C1—C7	122.3 (3)	N2—C12—H12A	109.5
C2—C1—C7	122.3 (3)	N2—C12—H12B	109.5
C1—C2—C3	121.6 (3)	H12A—C12—H12B	109.5
C1—C2—Cl1	118.5 (3)	N2—C12—H12C	109.5

C3—C2—Cl1	119.9 (3)	H12A—C12—H12C	109.5
C4—C3—C2	119.6 (3)	H12B—C12—H12C	109.5
C4—C3—H3A	120.2	O2—C13—N3	123.8 (2)
C2—C3—H3A	120.2	O2—C13—C9	130.5 (2)
C5—C4—C3	120.5 (3)	N3—C13—C9	105.7 (2)
C5—C4—H4A	119.8	C15—C14—C19	120.6 (3)
C3—C4—H4A	119.8	C15—C14—N3	120.6 (2)
C4—C5—C6	118.9 (3)	C19—C14—N3	118.7 (2)
C4—C5—H5A	120.6	C16—C15—C14	119.4 (2)
C6—C5—H5A	120.6	C16—C15—H15A	120.3
C5—C6—C1	124.1 (3)	C14—C15—H15A	120.3
C5—C6—Cl2	116.1 (3)	C17—C16—C15	120.5 (3)
C1—C6—Cl2	119.8 (2)	C17—C16—H16A	119.8
C1—C7—C8	114.5 (2)	C15—C16—H16A	119.8
C1—C7—H7A	108.6	C16—C17—C18	119.7 (3)
C8—C7—H7A	108.6	C16—C17—H17A	120.1
C1—C7—H7B	108.6	C18—C17—H17A	120.1
C8—C7—H7B	108.6	C19—C18—C17	120.6 (3)
H7A—C7—H7B	107.6	C19—C18—H18A	119.7
O1—C8—N1	123.4 (3)	C17—C18—H18A	119.7
O1—C8—C7	123.0 (2)	C18—C19—C14	119.1 (3)
N1—C8—C7	113.5 (2)	C18—C19—H19A	120.4
C10—C9—N1	128.8 (2)	C14—C19—H19A	120.4
C10—C9—C13	108.5 (2)		

C10—N2—N3—C13	−6.6 (3)	C13—C9—C10—N2	−4.7 (3)
C12—N2—N3—C13	−146.3 (2)	N1—C9—C10—C11	−9.5 (5)
C10—N2—N3—C14	−147.1 (2)	C13—C9—C10—C11	173.6 (3)
C12—N2—N3—C14	73.2 (3)	N3—N2—C10—C9	7.0 (3)
C6—C1—C2—C3	−2.4 (4)	C12—N2—C10—C9	142.5 (2)
C7—C1—C2—C3	175.4 (3)	N3—N2—C10—C11	−171.5 (2)
C6—C1—C2—Cl1	178.1 (2)	C12—N2—C10—C11	−36.0 (4)
C7—C1—C2—Cl1	−4.1 (4)	N2—N3—C13—O2	−175.1 (2)
C1—C2—C3—C4	1.4 (5)	C14—N3—C13—O2	−36.2 (4)
Cl1—C2—C3—C4	−179.1 (3)	N2—N3—C13—C9	3.7 (3)
C2—C3—C4—C5	0.1 (5)	C14—N3—C13—C9	142.6 (2)
C3—C4—C5—C6	−0.5 (5)	C10—C9—C13—O2	179.2 (3)
C4—C5—C6—C1	−0.7 (5)	N1—C9—C13—O2	2.1 (4)
C4—C5—C6—Cl2	179.2 (2)	C10—C9—C13—N3	0.5 (3)
C2—C1—C6—C5	2.1 (4)	N1—C9—C13—N3	−176.6 (2)
C7—C1—C6—C5	−175.7 (3)	C13—N3—C14—C15	−119.6 (3)
C2—C1—C6—Cl2	−177.8 (2)	N2—N3—C14—C15	15.9 (3)
C7—C1—C6—Cl2	4.5 (4)	C13—N3—C14—C19	57.4 (3)
C6—C1—C7—C8	−93.9 (3)	N2—N3—C14—C19	−167.0 (2)
C2—C1—C7—C8	88.5 (4)	C19—C14—C15—C16	−2.0 (4)
C9—N1—C8—O1	9.2 (4)	N3—C14—C15—C16	175.0 (2)
C9—N1—C8—C7	−168.3 (2)	C14—C15—C16—C17	−1.8 (4)
C1—C7—C8—O1	32.0 (4)	C15—C16—C17—C18	2.8 (4)
C1—C7—C8—N1	−150.6 (3)	C16—C17—C18—C19	0.1 (4)

C8—N1—C9—C10	−61.4 (4)	C17—C18—C19—C14	−3.8 (4)
C8—N1—C9—C13	115.1 (3)	C15—C14—C19—C18	4.8 (4)
N1—C9—C10—N2	172.2 (2)	N3—C14—C19—C18	−172.2 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O2^{i}	0.88	1.99	2.845 (3)	164
C7—H7*A*···O2^{i}	0.99	2.47	3.249 (3)	135
C12—H12*A*···O1^{ii}	0.98	2.43	3.104 (3)	126

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