Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

[1-(3-Chlorophenyl)-1*H*-1,2,3-triazol-4-yl]methanol hemihydrate

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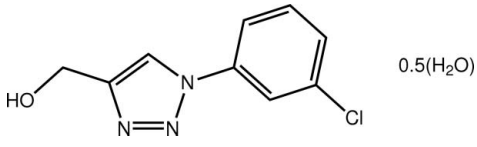
Received 7 October 2011; accepted 10 October 2011

Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.005 Å; R factor = 0.064; wR factor = 0.163; data-to-parameter ratio = 14.3.

The asymmetric unit of the title hydrate, $C_9H_8ClN_3O\cdot0.5H_2O$, comprises two independent 1,2,3-triazole molecules and a water molecule of crystallization. The dihedral angles between the six- and five-membered rings in the 1,2,3-triazole molecules are 12.71 (19) and 17.3 (2)°. The most significant different between them is found in the relative orientations of the terminal CH_2OH groups with one being close to perpendicular to the five-membered ring [N—C—C—O torsion angle = 82.2 (5)°], while in the other molecule, a notable deviation from a perpendicular disposition is found [torsion angle = −60.3 (5)°]. Supramolecular chains feature in the crystal packing sustained by O—H···(O,N) interactions along the *a*-axis direction. The chains are connected *via* C—H···N interactions and the resultant layers stack along the *b* axis.

Related literature

For background to the synthesis, biological activity and structures of 1,2,3-triazole derivatives, see: Boechat *et al.* (2010, 2011); Costa *et al.* (2006*a*,*b*); Ferreira *et al.* (2007); Jordão *et al.* (2009). For the synthesis, see: Boechat *et al.* (2011). For additional geometric analysis, see: Spek (2009).



Experimental

Crystal data

$C_9H_8ClN_3O\cdot0.5H_2O$
M_r = 218.64
Triclinic, $P\overline{1}$
a = 6.0078 (4) Å
b = 7.4897 (4) Å
c = 22.3145 (15) Å
α = 88.818 (4)°
β = 89.901 (2)°
γ = 80.493 (4)°
V = 990.07 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.36 mm^{-1}
T = 120 K
0.18 × 0.18 × 0.02 mm

Data collection

Bruker–Nonius APEX II CCD camera on κ-goniostat diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
T_{min} = 0.843, T_{max} = 1.000
10830 measured reflections
3909 independent reflections
2948 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.163
S = 1.00
3909 reflections
274 parameters
5 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1o···O2^{i}	0.84 (4)	1.82 (4)	2.651 (5)	170 (5)
O2—H2o···O1w	0.84 (6)	1.80 (5)	2.641 (5)	174 (7)
O1w—H1w···N3	0.84 (4)	2.00 (4)	2.837 (5)	172 (4)
O1w—H2w···O1^{ii}	0.84 (4)	1.95 (5)	2.663 (5)	142 (4)
C16—H16···O1w^{iii}	0.95	2.45	3.383 (5)	166
C7—H7···N6^{iv}	0.95	2.28	3.197 (5)	161

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

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997), *QMol* (Gans & Shalloway, 2001) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

The use of the EPSRC X-ray crystallographic service at the University of Southampton, England, and the valuable assistance of the staff there is gratefully acknowledged. JLW acknowledges support from CAPES and FAPEMIG (Brazil).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6439).

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supporting information

Acta Cryst. (2011). E**67**, o2934–o2935 [doi:10.1107/S1600536811041560]

[1-(3-Chlorophenyl)-1*H*-1,2,3-triazol-4-yl]methanol hemihydrate

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S1. Comment

Boechat and colleagues have been interested in the synthesis, biological activities and structures of 1,2,3-triazole derivatives for some time (Boechat *et al.*, 2010, 2011; Costa *et al.*, 2006*a*, 2006*b*; Ferreira *et al.*, 2007, Jordão *et al.*, 2009). Recently, they reported the synthesis and anti-mycobacterial activities of a number of 4-*R*-1-(*X*-phenyl)-triazole derivatives (Boechat *et al.*, 2011). The structure of one of the compounds investigated in that study, *i.e*. the title compound, (I), is now reported.

Two independent molecules of a 1,2,3-triazole derivative and a water molecule of solvation comprise the asymmetric unit of (I), Fig. 1. Geometrically, the two organic molecules are similar to each other with r.m.s. deviations for bond distances and angles being 0.0092 Å and 0.757°, respectively (Spek, 2009). From the overlay diagram, Fig. 2, it is evident that the independent molecules approximate mirror images. However, small twists between the five- and six-membered rings differ with the dihedral angles between their least-squares being 12.71 (19) and 17.3 (2)°, respectively, for the N1- and N4-containing molecules. More notable are the relative orientations of the terminal CH_2OH groups as seen in the values of the N3—C8—C9—O1 and N6—C17—C18—O2 torsion angles of 82.2 (5) and -60.3 (5)°, respectively.

The presence of a supramolecular chain along the *a* axis is the most prominent feature of the crystal packing, Fig. 3. These are mediated by O—H···O and O—H···N hydrogen bonds with additional stability afforded by C—H···O interactions, Table 1. Chains are connected into layers *via* C—H···N interactions, Table 1, and these stack along the *b* axis. The closest interactions between layers are of the type Cl···Cl, *i.e*. Cl1···Cl2^{i} = 3.4117 (15) Å for *i*: 2 - *x*, 1 - *y*, 1 - *z*.

S2. Experimental

The compound, obtained as published (Boechat *et al.*, 2011), was recrystallized from EtOH as a hemihydrate.

S3. Refinement

The C-bound H atoms were geometrically placed (C—H = 0.95–0.99 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C). The O—H H atoms were located from a difference map and refined with O—H = 0.84±0.01 Å, and with U_{iso}(H) = 1.5U_{eq}(O).

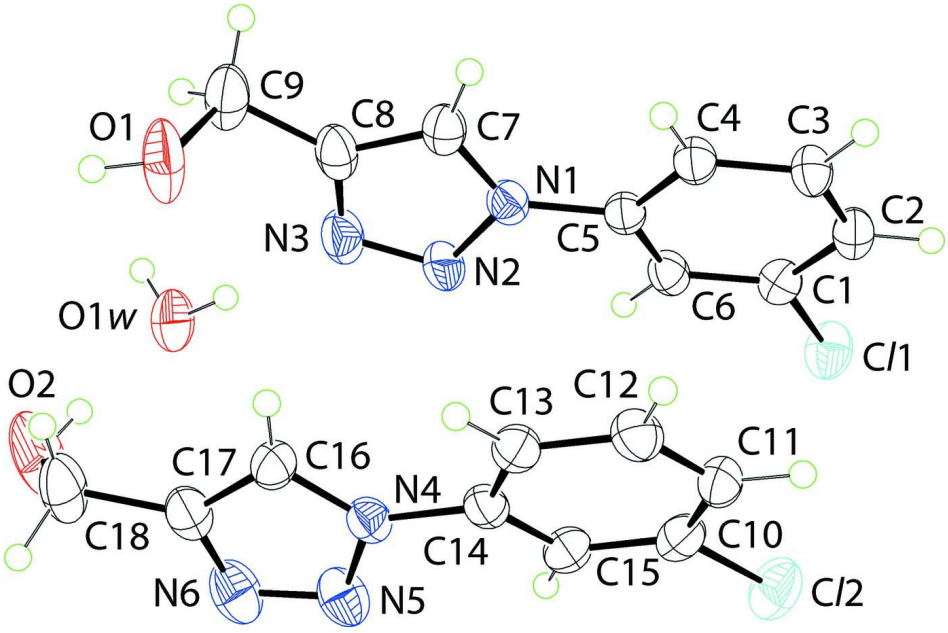

Figure 1

The molecular structures of the components comprising the asymmetric unit in (I) showing displacement ellipsoids at the 50% probability level.

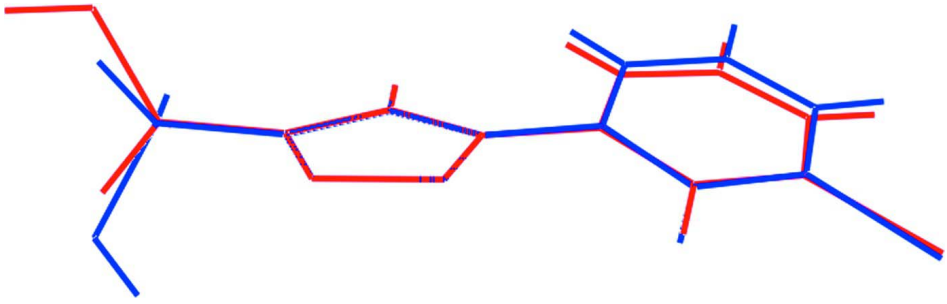

Figure 2

An overlay diagram of the two independent molecules in (I). The red and blue images illustrate the N1- and N3-containing molecules, respectively.

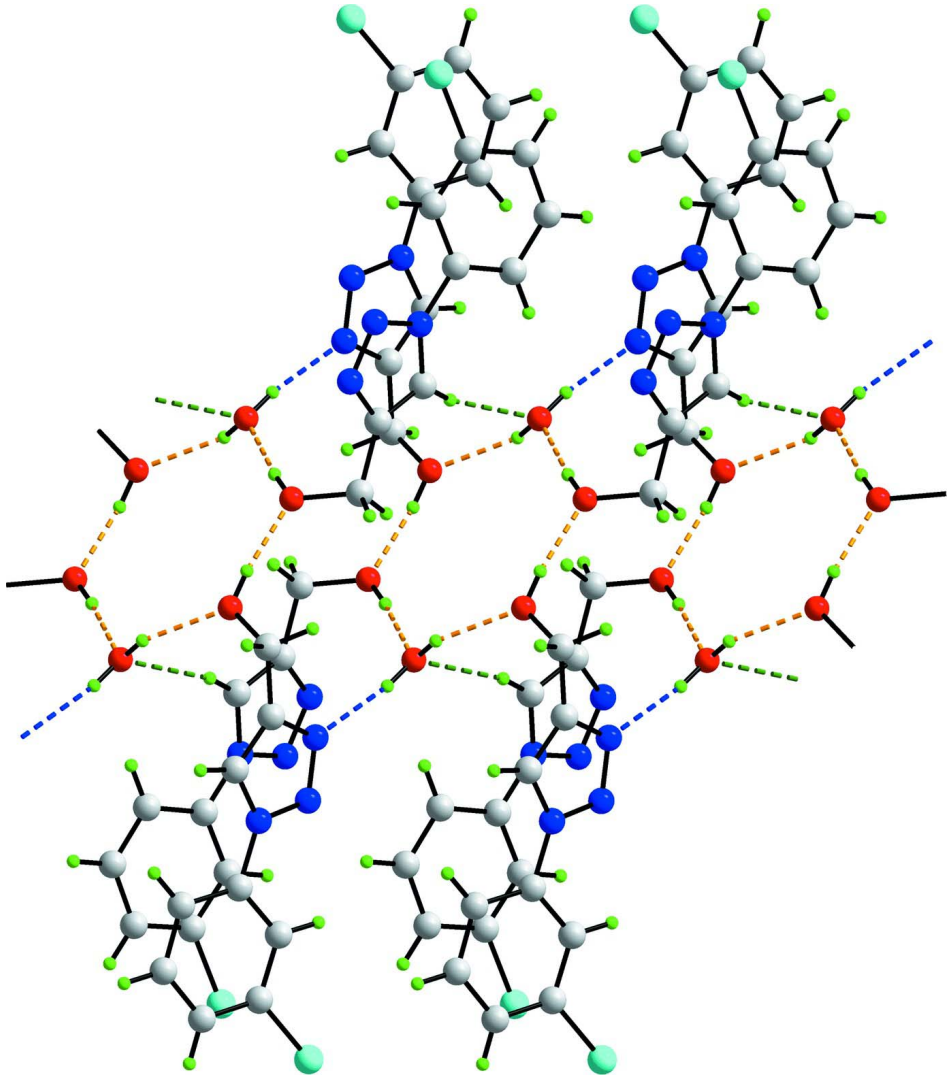

Figure 3

A view of the supramolecular chain aligned along the *a* axis in (I) mediated by O—H···O (red dashed lines), O—H···N (blue) hydrogen bonds and C—H···O interactions (green).

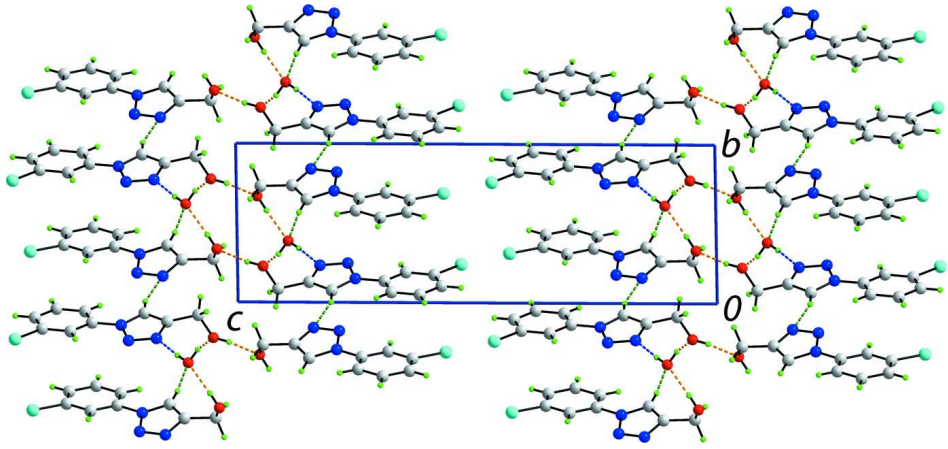

Figure 4

A view in projection down the *a* axis of the unit-cell contents in (I) showing the stacking of layers along the *b* axis. The O—H···O, O—H···N and C—H···O interactions are shown as orange, blue and green dashed lines, respectively.

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Crystal data

$C_9H_8ClN_3O·0.5H_2O$
M_r = 218.64
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 6.0078 (4) Å
b = 7.4897 (4) Å
c = 22.3145 (15) Å
α = 88.818 (4)°
β = 89.901 (2)°
γ = 80.493 (4)°
V = 990.07 (11) Å^3
Z = 4
$F(000)$ = 452
D_x = 1.467 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 19812 reflections
θ = 2.9–27.5°
μ = 0.36 mm^{-1}
T = 120 K
Plate, colourless
0.18 × 0.18 × 0.02 mm

Data collection

Bruker–Nonius APEX II CCD camera on κ-goniostat diffractometer
Radiation source: Bruker-Nonius FR591 rotating anode
10cm confocal mirrors monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
T_{min} = 0.843, T_{max} = 1.000
10830 measured reflections
3909 independent reflections
2948 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 26.5°, θ_{min} = 2.9°
h = −7→7
k = −9→9
l = −28→28

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.163
S = 1.00
3909 reflections
274 parameters
5 restraints
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

$w = 1/[\sigma^2(F_o^2) + (0.0446P)^2 + 2.5602P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.012$

$\Delta\rho_{max} = 0.41$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}

Special details

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.85344 (17)	0.75800 (15)	0.46687 (4)	0.0449 (3)
O1	0.5639 (6)	0.7737 (5)	0.05307 (13)	0.0595 (9)
H1O	0.629 (9)	0.747 (7)	0.0204 (13)	0.089*
N1	0.6411 (5)	0.8503 (4)	0.24523 (13)	0.0297 (6)
N2	0.8433 (5)	0.7528 (4)	0.23011 (14)	0.0386 (7)
N3	0.8614 (6)	0.7674 (4)	0.17193 (14)	0.0424 (8)
C1	0.6580 (6)	0.8250 (5)	0.41004 (15)	0.0304 (7)
C2	0.4384 (6)	0.8954 (5)	0.42488 (16)	0.0343 (8)
H2	0.3932	0.9055	0.4657	0.041*
C3	0.2852 (6)	0.9509 (5)	0.37926 (15)	0.0331 (8)
H3	0.1338	1.0005	0.3889	0.040*
C4	0.3494 (6)	0.9352 (5)	0.31987 (16)	0.0317 (8)
H4	0.2426	0.9724	0.2889	0.038*
C5	0.5708 (6)	0.8647 (4)	0.30588 (15)	0.0280 (7)
C6	0.7280 (6)	0.8092 (5)	0.35095 (15)	0.0314 (8)
H6	0.8801	0.7614	0.3414	0.038*
C7	0.5315 (6)	0.9254 (5)	0.19577 (15)	0.0322 (8)
H7	0.3870	0.9992	0.1940	0.039*
C8	0.6716 (7)	0.8731 (5)	0.14894 (16)	0.0381 (9)
C9	0.6412 (8)	0.9160 (6)	0.08392 (17)	0.0484 (11)
H9A	0.5309	1.0289	0.0784	0.058*
H9B	0.7867	0.9368	0.0665	0.058*
Cl2	0.7137 (2)	0.31120 (15)	0.43211 (4)	0.0519 (3)
O2	1.1922 (7)	0.3320 (5)	0.04279 (18)	0.0843 (14)
H2O	1.219 (12)	0.422 (6)	0.062 (3)	0.126*
N4	0.7744 (5)	0.2978 (4)	0.20400 (13)	0.0306 (6)
N5	0.9702 (5)	0.1798 (5)	0.21008 (15)	0.0433 (8)
N6	1.0590 (6)	0.1604 (5)	0.15647 (16)	0.0485 (9)
C10	0.5956 (6)	0.3531 (5)	0.36144 (16)	0.0348 (8)
C11	0.3706 (6)	0.4305 (5)	0.35577 (16)	0.0359 (8)
H11	0.2793	0.4587	0.3902	0.043*
C12	0.2826 (6)	0.4657 (5)	0.29895 (17)	0.0389 (9)

H12	0.1293	0.5210	0.2943	0.047*
C13	0.4137 (6)	0.4217 (5)	0.24830 (16)	0.0318 (8)
H13	0.3506	0.4445	0.2093	0.038*
C14	0.6367 (6)	0.3444 (4)	0.25557 (16)	0.0309 (8)
C15	0.7315 (6)	0.3090 (5)	0.31195 (16)	0.0323 (8)
H15	0.8855	0.2558	0.3166	0.039*
C16	0.7421 (6)	0.3525 (5)	0.14617 (16)	0.0350 (8)
H16	0.6188	0.4348	0.1298	0.042*
C17	0.9245 (7)	0.2643 (5)	0.11626 (18)	0.0395 (9)
C18	0.9826 (8)	0.2697 (6)	0.05057 (19)	0.0538 (12)
H18A	0.9928	0.1471	0.0339	0.065*
H18B	0.8623	0.3516	0.0287	0.065*
O1W	1.2489 (5)	0.6147 (4)	0.10634 (13)	0.0491 (7)
H1W	1.143 (6)	0.661 (6)	0.1286 (19)	0.074*
H2W	1.293 (8)	0.698 (5)	0.086 (2)	0.074*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0387 (5)	0.0620 (7)	0.0332 (5)	−0.0063 (4)	−0.0052 (4)	0.0013 (4)
O1	0.081 (2)	0.077 (2)	0.0334 (15)	−0.0501 (19)	0.0214 (15)	−0.0252 (15)
N1	0.0308 (16)	0.0279 (15)	0.0314 (15)	−0.0076 (12)	0.0057 (12)	−0.0036 (12)
N2	0.0380 (18)	0.0384 (18)	0.0380 (17)	−0.0016 (14)	0.0155 (14)	−0.0037 (13)
N3	0.049 (2)	0.0433 (19)	0.0375 (18)	−0.0135 (15)	0.0174 (16)	−0.0073 (14)
C1	0.0303 (18)	0.0333 (19)	0.0288 (17)	−0.0085 (14)	−0.0026 (14)	−0.0010 (14)
C2	0.037 (2)	0.039 (2)	0.0283 (18)	−0.0112 (16)	0.0055 (16)	−0.0051 (15)
C3	0.0289 (18)	0.039 (2)	0.0310 (18)	−0.0040 (15)	0.0073 (15)	−0.0030 (15)
C4	0.0339 (19)	0.0316 (19)	0.0298 (18)	−0.0061 (14)	0.0050 (15)	−0.0024 (14)
C5	0.0308 (18)	0.0259 (17)	0.0283 (17)	−0.0074 (13)	0.0036 (14)	−0.0025 (13)
C6	0.0280 (18)	0.0317 (19)	0.0348 (19)	−0.0056 (14)	0.0070 (15)	−0.0043 (14)
C7	0.0345 (19)	0.0354 (19)	0.0290 (18)	−0.0120 (15)	0.0024 (15)	−0.0039 (14)
C8	0.048 (2)	0.038 (2)	0.0327 (19)	−0.0193 (17)	0.0104 (17)	−0.0109 (16)
C9	0.070 (3)	0.051 (3)	0.032 (2)	−0.032 (2)	0.014 (2)	−0.0089 (18)
Cl2	0.0633 (7)	0.0630 (7)	0.0319 (5)	−0.0187 (5)	−0.0054 (5)	0.0050 (4)
O2	0.093 (3)	0.094 (3)	0.085 (3)	−0.067 (2)	0.063 (2)	−0.049 (2)
N4	0.0293 (15)	0.0294 (15)	0.0333 (16)	−0.0048 (12)	0.0040 (12)	−0.0042 (12)
N5	0.0298 (17)	0.050 (2)	0.047 (2)	0.0020 (14)	0.0020 (15)	−0.0105 (15)
N6	0.0359 (19)	0.057 (2)	0.053 (2)	−0.0086 (16)	0.0100 (17)	−0.0177 (17)
C10	0.043 (2)	0.034 (2)	0.0289 (18)	−0.0136 (16)	−0.0044 (16)	0.0042 (14)
C11	0.041 (2)	0.036 (2)	0.0318 (19)	−0.0101 (16)	0.0087 (16)	−0.0011 (15)
C12	0.034 (2)	0.036 (2)	0.045 (2)	−0.0018 (16)	0.0087 (17)	−0.0016 (16)
C13	0.0333 (19)	0.0312 (19)	0.0316 (18)	−0.0075 (14)	−0.0006 (15)	−0.0011 (14)
C14	0.0329 (19)	0.0259 (18)	0.0355 (19)	−0.0087 (14)	0.0080 (15)	−0.0039 (14)
C15	0.0308 (19)	0.0333 (19)	0.0340 (19)	−0.0086 (14)	−0.0009 (15)	0.0027 (14)
C16	0.041 (2)	0.034 (2)	0.0316 (19)	−0.0113 (16)	0.0063 (16)	−0.0002 (15)
C17	0.044 (2)	0.038 (2)	0.042 (2)	−0.0190 (17)	0.0149 (18)	−0.0105 (17)
C18	0.061 (3)	0.063 (3)	0.046 (2)	−0.033 (2)	0.026 (2)	−0.019 (2)
O1W	0.0453 (17)	0.065 (2)	0.0381 (16)	−0.0109 (14)	0.0155 (13)	−0.0064 (14)

Geometric parameters (Å, º)

Cl1—C1	1.739 (4)	O2—C18	1.423 (5)
O1—C9	1.422 (5)	O2—H2O	0.840 (10)
O1—H1O	0.839 (10)	N4—C16	1.350 (4)
N1—C7	1.350 (4)	N4—N5	1.355 (4)
N1—N2	1.356 (4)	N4—C14	1.431 (4)
N1—C5	1.418 (4)	N5—N6	1.310 (5)
N2—N3	1.307 (4)	N6—C17	1.353 (5)
N3—C8	1.370 (5)	C10—C11	1.385 (5)
C1—C2	1.380 (5)	C10—C15	1.385 (5)
C1—C6	1.385 (5)	C11—C12	1.378 (5)
C2—C3	1.384 (5)	C11—H11	0.9500
C2—H2	0.9500	C12—C13	1.390 (5)
C3—C4	1.382 (5)	C12—H12	0.9500
C3—H3	0.9500	C13—C14	1.377 (5)
C4—C5	1.385 (5)	C13—H13	0.9500
C4—H4	0.9500	C14—C15	1.384 (5)
C5—C6	1.390 (5)	C15—H15	0.9500
C6—H6	0.9500	C16—C17	1.364 (5)
C7—C8	1.363 (5)	C16—H16	0.9500
C7—H7	0.9500	C17—C18	1.507 (5)
C8—C9	1.485 (5)	C18—H18A	0.9900
C9—H9A	0.9900	C18—H18B	0.9900
C9—H9B	0.9900	O1W—H1W	0.840 (10)
Cl2—C10	1.731 (4)	O1W—H2W	0.838 (10)
C9—O1—H1O	115 (4)	C16—N4—N5	110.3 (3)
C7—N1—N2	110.3 (3)	C16—N4—C14	130.2 (3)
C7—N1—C5	128.6 (3)	N5—N4—C14	119.5 (3)
N2—N1—C5	121.1 (3)	N6—N5—N4	106.6 (3)
N3—N2—N1	106.9 (3)	N5—N6—C17	109.9 (3)
N2—N3—C8	109.7 (3)	C11—C10—C15	121.9 (3)
C2—C1—C6	121.7 (3)	C11—C10—Cl2	119.7 (3)
C2—C1—Cl1	119.3 (3)	C15—C10—Cl2	118.5 (3)
C6—C1—Cl1	119.0 (3)	C12—C11—C10	118.3 (3)
C1—C2—C3	118.8 (3)	C12—C11—H11	120.8
C1—C2—H2	120.6	C10—C11—H11	120.8
C3—C2—H2	120.6	C11—C12—C13	121.3 (4)
C4—C3—C2	120.9 (3)	C11—C12—H12	119.4
C4—C3—H3	119.6	C13—C12—H12	119.4
C2—C3—H3	119.6	C14—C13—C12	118.9 (3)
C3—C4—C5	119.5 (3)	C14—C13—H13	120.6
C3—C4—H4	120.3	C12—C13—H13	120.6
C5—C4—H4	120.3	C13—C14—C15	121.4 (3)
C6—C5—C4	120.7 (3)	C13—C14—N4	119.7 (3)
C6—C5—N1	119.0 (3)	C15—C14—N4	118.8 (3)
C4—C5—N1	120.4 (3)	C14—C15—C10	118.2 (3)

C5—C6—C1	118.5 (3)	C14—C15—H15	120.9
C5—C6—H6	120.7	C10—C15—H15	120.9
C1—C6—H6	120.7	N4—C16—C17	105.2 (3)
N1—C7—C8	105.6 (3)	N4—C16—H16	127.4
N1—C7—H7	127.2	C17—C16—H16	127.4
C8—C7—H7	127.2	N6—C17—C16	108.0 (3)
C7—C8—N3	107.5 (3)	N6—C17—C18	122.0 (4)
C7—C8—C9	129.8 (4)	C16—C17—C18	129.9 (4)
N3—C8—C9	122.7 (3)	O2—C18—C17	109.9 (4)
O1—C9—C8	111.6 (3)	O2—C18—H18A	109.7
O1—C9—H9A	109.3	C17—C18—H18A	109.7
C8—C9—H9A	109.3	O2—C18—H18B	109.7
O1—C9—H9B	109.3	C17—C18—H18B	109.7
C8—C9—H9B	109.3	H18A—C18—H18B	108.2
H9A—C9—H9B	108.0	H1W—O1W—H2W	109 (4)
C18—O2—H2O	120 (5)		

C7—N1—N2—N3	0.5 (4)	C16—N4—N5—N6	−0.2 (4)
C5—N1—N2—N3	−179.0 (3)	C14—N4—N5—N6	179.2 (3)
N1—N2—N3—C8	−0.3 (4)	N4—N5—N6—C17	0.3 (4)
C6—C1—C2—C3	0.1 (5)	C15—C10—C11—C12	−0.7 (5)
Cl1—C1—C2—C3	179.0 (3)	Cl2—C10—C11—C12	178.7 (3)
C1—C2—C3—C4	0.5 (5)	C10—C11—C12—C13	1.3 (5)
C2—C3—C4—C5	−0.7 (5)	C11—C12—C13—C14	−1.1 (5)
C3—C4—C5—C6	0.3 (5)	C12—C13—C14—C15	0.4 (5)
C3—C4—C5—N1	−178.9 (3)	C12—C13—C14—N4	179.9 (3)
C7—N1—C5—C6	−166.4 (3)	C16—N4—C14—C13	17.2 (5)
N2—N1—C5—C6	12.9 (5)	N5—N4—C14—C13	−162.1 (3)
C7—N1—C5—C4	12.8 (5)	C16—N4—C14—C15	−163.2 (3)
N2—N1—C5—C4	−167.9 (3)	N5—N4—C14—C15	17.4 (5)
C4—C5—C6—C1	0.3 (5)	C13—C14—C15—C10	0.1 (5)
N1—C5—C6—C1	179.5 (3)	N4—C14—C15—C10	−179.4 (3)
C2—C1—C6—C5	−0.5 (5)	C11—C10—C15—C14	0.0 (5)
Cl1—C1—C6—C5	−179.4 (3)	Cl2—C10—C15—C14	−179.4 (3)
N2—N1—C7—C8	−0.4 (4)	N5—N4—C16—C17	0.1 (4)
C5—N1—C7—C8	179.0 (3)	C14—N4—C16—C17	−179.3 (3)
N1—C7—C8—N3	0.2 (4)	N5—N6—C17—C16	−0.3 (4)
N1—C7—C8—C9	−179.4 (3)	N5—N6—C17—C18	−179.8 (3)
N2—N3—C8—C7	0.1 (4)	N4—C16—C17—N6	0.1 (4)
N2—N3—C8—C9	179.7 (3)	N4—C16—C17—C18	179.6 (4)
C7—C8—C9—O1	−98.3 (5)	N6—C17—C18—O2	−60.3 (5)
N3—C8—C9—O1	82.2 (5)	C16—C17—C18—O2	120.2 (5)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1o···O2^{i}	0.84 (4)	1.82 (4)	2.651 (5)	170 (5)
O2—H2o···O1w	0.84 (6)	1.80 (5)	2.641 (5)	174 (7)

O1w—H1w···N3	0.84 (4)	2.00 (4)	2.837 (5)	172 (4)
O1w—H2w···O1^{ii}	0.84 (4)	1.95 (5)	2.663 (5)	142 (4)
C16—H16···O1w^{iii}	0.95	2.45	3.383 (5)	166
C7—H7···N6^{iv}	0.95	2.28	3.197 (5)	161

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