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[1-(2,5-Dichloroanilino)-5-methyl-1*H*-1,2,3-triazol-4-yl]methanol

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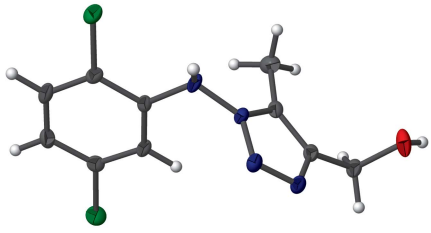
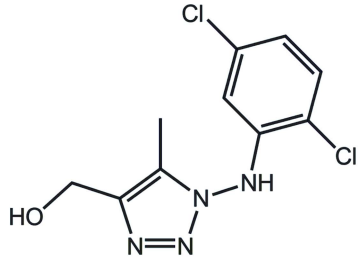
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{10}H_{10}Cl_2N_4O$, the hydroxy group and benzene ring are disposed to opposite sides of the central 1,2,3-triazolyl ring. The dihedral angle between the five- and six-membered rings is 87.51 (12)°, and the C—O bond of the hydroxy group lies almost normal to the plane of the 5-membered ring [N—C—C—O = −93.2 (2)°]. An intramolecular amino-N—H···Cl hydrogen bond is noted. In the extended structure, supramolecular layers in the *ab* plane are formed *via* hydroxy-O—H···N(ring) and amine-N—H···O(hydroxy) hydrogen bonds. The layers are connected along the *c* axis by π–π contacts between benzene rings [inter-centroid distance = 3.7789 (13) Å] and by C—Cl···π interactions.

3D view



Chemical scheme



Structure description

1,2,3-Triazole derivatives attract continuing interest as a result of their biological activities (Dehaen & Bakulev, 2014). Diseases that have been evaluated recently include tuberculosis (Jordão *et al.*, 2011), and the susceptibility of Cantagalo virus to 1,2,3-triazoles has also been investigated (Jordão *et al.*, 2009). These studies have provided a number of crystals enabling systematic studies of the influence of the electronegativity of aryl-bound substituents upon crystal packing patterns (Cunha *et al.*, 2013; Seth *et al.*, 2015).

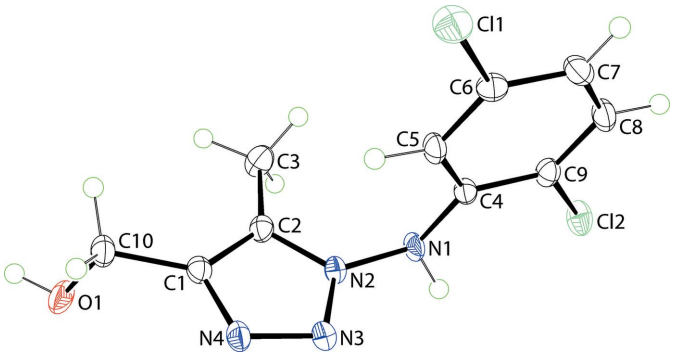


Figure 1
The molecular structure of the title compound showing the atom-labelling scheme and displacement ellipsoids at the 50% probability level.

The central 1,2,3-triazolyl ring (r.m.s. deviation = 0.006 Å) in the title compound, Fig. 1, is flanked by C1-bound hydroxymethyl and N2-bound amino-2,5-dichlorobenzene substituents which lie to opposite sides of the ring. The C—O grouping of the hydroxyl group lies almost normal to the ring with the N4—C1—C10—O1 torsion angle being −93.2 (2)°. The dihedral angle between the triazolyl and benzene rings is 87.51 (12)°, with the latter being almost perpendicular, forming a N2—N1—C4—C5 torsion angle of −8.9 (3)°. This alignment allows for the formation of an intramolecular amino-N—H···Cl hydrogen bond, Table 1.

In the molecular packing, the hydroxy group is pivotal in the hydrogen-bonding scheme, forming donor hydroxy-O—H···N(ring) and acceptor amine-N—H···O(hydroxy) interactions, Table 1. The latter interactions assemble molecules into dimers and these are in turn connected into supramolecular layers in the *ab* plane by the former interactions. The connections between layers are afforded by inter-digitating benzene rings *via* π—π contacts [inter-centroid distance = 3.7789 (13) Å for symmetry operation $1-x, -\frac{1}{2}+y, \frac{3}{2}-z$] and C—Cl···$\pi$ interactions, Table 1 and Fig. 2.

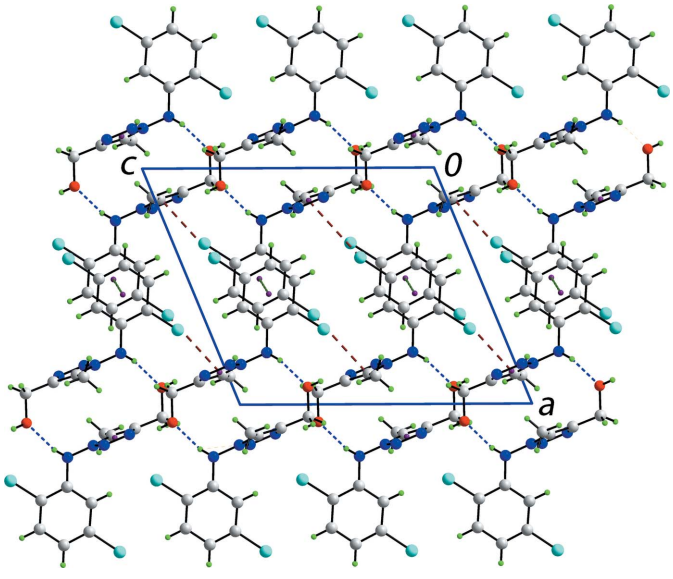


Figure 2
A view of the unit cell contents of the title compound shown in projection down the *b* axis. The O—H···O, N—H···O, π—π and C—Cl···π interactions are shown as orange, blue, green and brown dashed lines, respectively.

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

*Cg*1 is the centroid of the C4–C9 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*···Cl2	0.87 (2)	2.67 (2)	2.9530 (19)	100 (2)
O1—H1*O*···N4^{i}	0.84 (2)	2.01 (2)	2.836 (2)	169 (2)
N1—H1*N*···O1^{ii}	0.87 (2)	2.01 (2)	2.848 (3)	165 (2)
C6—Cl1···*Cg*1^{iii}	1.74 (1)	3.73 (1)	5.411 (3)	161 (1)

Symmetry codes: (i) $-x+2, y-\frac{1}{2}, -z+\frac{5}{2}$; (ii) $-x+2, -y+1, -z+2$; (iii) $-x+1, -y+1, -z+2$.

Synthesis and crystallization

A solution of the desired 4-carbethoxy-triazole (Cunha *et al.*, 2013) (1.00 mmol) in anhydrous THF (5 ml) was added dropwise to a suspension of $LiAlH_4$ (2 mmol) in anhydrous THF (10 ml) under a nitrogen atmosphere at 0°C. The reaction mixture was stirred at room temperature for 2 h, water (10 ml) was added, the aqueous layer acidified to pH 1 with 1 *M* HCl, and extracted with CH_2Cl_2 (3 ×). The organic

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{10}H_{10}Cl_2N_4O$
M_r	273.12
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	120
a, *b*, *c* (Å)	12.1802 (5), 7.3646 (4), 13.9001 (8)
β (°)	112.276 (3)
V (Å^3)	1153.81 (11)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	0.55
Crystal size (mm)	0.26 × 0.18 × 0.16
Data collection	
Diffractometer	Bruker–Nonius 95mm CCD camera on κ-goniostat diffractometer
Absorption correction	Multi-scan (*SADABS*; Sheldrick, 2003)
T_{min}, T_{max}	0.768, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12461, 2645, 1963
R_{int}	0.062
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.649
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.043, 0.117, 1.06
No. of reflections	2645
No. of parameters	161
No. of restraints	2
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.33, −0.40

Computer programs: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012), *DIAMOND* (Brandenburg, 2006), *publCIF* (Westrip, 2010).

extracts were combined, dried with Na_2SO_4, and concentrated under reduced pressure. The resulting residue was washed with hexane/dichloromethane (3:1) and dried under vacuum. 44% yield. Crystals were obtained from the slow evaporation of its methanol solution. M.p. 197°C. IR (KBr) ν_{max} (cm^{-1}): 3184 (N—H); 3096 (O—H). ^{1}H NMR (300 MHz, DMSO-d_6) δ: 2.18 (*s*, 3H, CH_3), 4.55 (*d*, 2H, *J* = 5.6 Hz, CH_2OH), 5.19 (*t*, 1H, *J* = 5.6 Hz, CH_2OH), 5.80 (*d*, 1H, *J* = 2.4 Hz, H5), 7.00 (*dd*, 1H, *J* = 2.4 & 8.5 Hz, H7), 7.50 (*d*, 1H, *J* = 8.5 Hz, H8), 10.21 (*s*, 1H, NH). ^{13}C NMR (75 MHz, DMSO-d_6) δ: 6.8 (CH_3), 54.8 (CH_2), 112.4 (C5), 116.4 (C6), 121.5 (C7), 131.3 (C8), 132.0 (C9), 132.7 (C1or C2), 143.6 (C1 or C2), 143.7 (C4). Anal. calcd. For $C_{10}H_{10}Cl_2N4O$: C, 43.98; H, 3.69; N, 20.51. Found: C, 44.01; H, 3.72; N, 20.09.

Refinement

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

Acknowledgements

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full crystallographic data

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Crystal data

$C_{10}H_{10}Cl_2N_4O$
M_r = 273.12
Monoclinic, $P2_1/c$
a = 12.1802 (5) Å
b = 7.3646 (4) Å
c = 13.9001 (8) Å
β = 112.276 (3)°
V = 1153.81 (11) Å^3
Z = 4
$F(000)$ = 560
D_x = 1.572 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71069 Å
Cell parameters from 2686 reflections
θ = 2.9–27.5°
μ = 0.55 mm^{-1}
T = 120 K
Block, colourless
0.26 × 0.18 × 0.16 mm

Data collection

Bruker-Nonius 95mm CCD camera on κ-goniostat diffractometer
Radiation source: Bruker-Nonius FR591 rotating anode
Graphite monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ & ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.768, T_{max} = 1.000
12461 measured reflections
2645 independent reflections
1963 reflections with $I > 2\sigma(I)$
R_{int} = 0.062
θ_{max} = 27.5°, θ_{min} = 3.0°
h = −15→14
k = −9→9
l = −18→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.117
S = 1.06
2645 reflections
161 parameters
2 restraints
Hydrogen site location: mixed
$w = 1/[\sigma^2(F_o^2) + (0.0528P)^2 + 0.5445P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

Special details

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.37932 (5)	0.38765 (8)	0.87969 (5)	0.02943 (19)
Cl2	0.68215 (5)	0.39438 (8)	0.60698 (4)	0.02549 (18)
O1	1.07381 (14)	0.3879 (2)	1.25648 (13)	0.0289 (4)
H1O	1.098 (2)	0.319 (3)	1.3086 (16)	0.043*
N1	0.78023 (15)	0.4396 (3)	0.83509 (14)	0.0188 (4)
H1N	0.8125 (19)	0.503 (3)	0.8004 (17)	0.023*
N2	0.82967 (15)	0.4789 (2)	0.94015 (13)	0.0163 (4)
N3	0.83152 (15)	0.6498 (2)	0.97786 (14)	0.0190 (4)
N4	0.87624 (15)	0.6334 (2)	1.07929 (14)	0.0190 (4)
C1	0.90092 (17)	0.4551 (3)	1.10644 (16)	0.0177 (5)
C2	0.87186 (17)	0.3534 (3)	1.01696 (17)	0.0175 (5)
C3	0.8799 (2)	0.1582 (3)	0.99578 (19)	0.0249 (5)
H3A	0.8016	0.1136	0.9502	0.037*
H3B	0.9070	0.0906	1.0614	0.037*
H3C	0.9364	0.1410	0.9617	0.037*
C4	0.65537 (18)	0.4209 (3)	0.79153 (16)	0.0164 (4)
C5	0.58710 (19)	0.4161 (3)	0.85238 (17)	0.0190 (5)
H5	0.6234	0.4282	0.9258	0.023*
C6	0.46531 (19)	0.3934 (3)	0.80412 (18)	0.0195 (5)
C7	0.40899 (19)	0.3747 (3)	0.69811 (18)	0.0227 (5)
H7	0.3252	0.3615	0.6670	0.027*
C8	0.4772 (2)	0.3757 (3)	0.63790 (18)	0.0231 (5)
H8	0.4404	0.3614	0.5647	0.028*
C9	0.59873 (19)	0.3976 (3)	0.68423 (17)	0.0185 (5)
C10	0.94792 (19)	0.3937 (3)	1.21697 (17)	0.0211 (5)
H10A	0.9215	0.4782	1.2592	0.025*
H10B	0.9164	0.2715	1.2216	0.025*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0241 (3)	0.0385 (4)	0.0300 (4)	−0.0026 (2)	0.0151 (3)	−0.0009 (3)
Cl2	0.0269 (3)	0.0356 (4)	0.0139 (3)	0.0017 (2)	0.0077 (2)	−0.0017 (2)
O1	0.0178 (8)	0.0412 (11)	0.0218 (9)	−0.0036 (7)	0.0011 (7)	0.0160 (7)
N1	0.0197 (9)	0.0277 (10)	0.0083 (9)	−0.0043 (7)	0.0045 (7)	−0.0016 (7)
N2	0.0177 (8)	0.0190 (10)	0.0111 (9)	−0.0001 (7)	0.0041 (7)	−0.0008 (7)
N3	0.0193 (9)	0.0213 (10)	0.0143 (10)	−0.0011 (7)	0.0038 (7)	−0.0008 (7)
N4	0.0195 (9)	0.0230 (10)	0.0128 (10)	−0.0006 (7)	0.0043 (7)	−0.0009 (7)
C1	0.0149 (10)	0.0225 (11)	0.0155 (11)	−0.0018 (8)	0.0055 (8)	0.0003 (9)
C2	0.0147 (10)	0.0228 (12)	0.0151 (11)	−0.0004 (8)	0.0060 (8)	0.0020 (9)
C3	0.0324 (13)	0.0213 (12)	0.0226 (13)	0.0030 (9)	0.0122 (10)	0.0026 (10)
C4	0.0161 (10)	0.0163 (10)	0.0142 (11)	0.0004 (8)	0.0030 (8)	0.0005 (8)
C5	0.0211 (11)	0.0224 (12)	0.0114 (11)	−0.0003 (8)	0.0037 (9)	−0.0013 (8)
C6	0.0193 (11)	0.0182 (11)	0.0224 (12)	−0.0003 (8)	0.0095 (9)	−0.0004 (9)
C7	0.0170 (11)	0.0217 (12)	0.0242 (13)	−0.0011 (8)	0.0020 (9)	−0.0015 (9)

C8	0.0248 (12)	0.0238 (12)	0.0143 (11)	0.0000 (9)	0.0002 (9)	−0.0013 (9)
C9	0.0232 (11)	0.0176 (11)	0.0146 (11)	0.0014 (8)	0.0070 (9)	−0.0002 (8)
C10	0.0201 (11)	0.0281 (13)	0.0140 (11)	−0.0008 (9)	0.0055 (9)	0.0014 (9)

Geometric parameters (Å, º)

Cl1—C6	1.742 (2)	C3—H3A	0.9800
Cl2—C9	1.736 (2)	C3—H3B	0.9800
O1—C10	1.420 (3)	C3—H3C	0.9800
O1—H1O	0.839 (10)	C4—C5	1.393 (3)
N1—N2	1.383 (2)	C4—C9	1.396 (3)
N1—C4	1.414 (3)	C5—C6	1.387 (3)
N1—H1N	0.866 (10)	C5—H5	0.9500
N2—C2	1.357 (3)	C6—C7	1.376 (3)
N2—N3	1.361 (3)	C7—C8	1.385 (3)
N3—N4	1.310 (3)	C7—H7	0.9500
N4—C1	1.368 (3)	C8—C9	1.382 (3)
C1—C2	1.378 (3)	C8—H8	0.9500
C1—C10	1.492 (3)	C10—H10A	0.9900
C2—C3	1.478 (3)	C10—H10B	0.9900
C10—O1—H1O	109 (2)	C9—C4—N1	119.01 (18)
N2—N1—C4	116.08 (16)	C6—C5—C4	119.0 (2)
N2—N1—H1N	111.5 (16)	C6—C5—H5	120.5
C4—N1—H1N	117.1 (16)	C4—C5—H5	120.5
C2—N2—N3	112.40 (17)	C7—C6—C5	122.5 (2)
C2—N2—N1	124.87 (18)	C7—C6—Cl1	118.26 (16)
N3—N2—N1	122.50 (17)	C5—C6—Cl1	119.24 (17)
N4—N3—N2	105.56 (16)	C6—C7—C8	118.48 (19)
N3—N4—C1	110.12 (17)	C6—C7—H7	120.8
N4—C1—C2	108.56 (19)	C8—C7—H7	120.8
N4—C1—C10	122.24 (19)	C9—C8—C7	120.1 (2)
C2—C1—C10	129.2 (2)	C9—C8—H8	120.0
N2—C2—C1	103.36 (18)	C7—C8—H8	120.0
N2—C2—C3	122.65 (19)	C8—C9—C4	121.3 (2)
C1—C2—C3	134.0 (2)	C8—C9—Cl2	119.02 (17)
C2—C3—H3A	109.5	C4—C9—Cl2	119.63 (16)
C2—C3—H3B	109.5	O1—C10—C1	110.11 (17)
H3A—C3—H3B	109.5	O1—C10—H10A	109.6
C2—C3—H3C	109.5	C1—C10—H10A	109.6
H3A—C3—H3C	109.5	O1—C10—H10B	109.6
H3B—C3—H3C	109.5	C1—C10—H10B	109.6
C5—C4—C9	118.58 (19)	H10A—C10—H10B	108.2
C5—C4—N1	122.34 (19)		
C4—N1—N2—C2	93.4 (2)	N2—N1—C4—C9	174.27 (18)
C4—N1—N2—N3	−80.6 (2)	C9—C4—C5—C6	−1.7 (3)
C2—N2—N3—N4	0.6 (2)	N1—C4—C5—C6	−178.6 (2)

N1—N2—N3—N4	175.36 (16)	C4—C5—C6—C7	0.2 (3)
N2—N3—N4—C1	−1.0 (2)	C4—C5—C6—Cl1	−179.89 (16)
N3—N4—C1—C2	1.0 (2)	C5—C6—C7—C8	1.1 (3)
N3—N4—C1—C10	−177.30 (18)	Cl1—C6—C7—C8	−178.78 (17)
N3—N2—C2—C1	0.0 (2)	C6—C7—C8—C9	−0.9 (3)
N1—N2—C2—C1	−174.61 (17)	C7—C8—C9—C4	−0.7 (3)
N3—N2—C2—C3	−179.43 (18)	C7—C8—C9—Cl2	178.92 (17)
N1—N2—C2—C3	6.0 (3)	C5—C4—C9—C8	2.0 (3)
N4—C1—C2—N2	−0.6 (2)	N1—C4—C9—C8	178.94 (19)
C10—C1—C2—N2	177.57 (19)	C5—C4—C9—Cl2	−177.60 (16)
N4—C1—C2—C3	178.7 (2)	N1—C4—C9—Cl2	−0.6 (3)
C10—C1—C2—C3	−3.1 (4)	N4—C1—C10—O1	−93.2 (2)
N2—N1—C4—C5	−8.9 (3)	C2—C1—C10—O1	88.9 (3)

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C4–C9 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*···Cl2	0.87 (2)	2.67 (2)	2.9530 (19)	100 (2)
O1—H1*O*···N4^{i}	0.84 (2)	2.01 (2)	2.836 (2)	169 (2)
N1—H1*N*···O1^{ii}	0.87 (2)	2.01 (2)	2.848 (3)	165 (2)
C6—Cl1···*Cg*1^{iii}	1.74 (1)	3.73 (1)	5.411 (3)	161 (1)

Symmetry codes: (i) −*x*+2, *y*−1/2, −*z*+5/2; (ii) −*x*+2, −*y*+1, −*z*+2; (iii) −*x*+1, −*y*+1, −*z*+2.