

Acta Crystallographica Section E

## Structure Reports

Online

ISSN 1600-5368

## 1-(3,5-Dichlorophenyl)-1H-1,2,3,4-tetrazole

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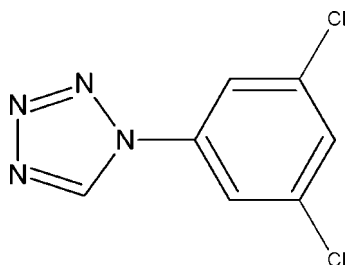
Received 8 January 2012; accepted 11 January 2012

Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å;  $R$  factor = 0.057;  $wR$  factor = 0.114; data-to-parameter ratio = 14.3.

In the title compound,  $\text{C}_7\text{H}_4\text{Cl}_2\text{N}_4$ , the dihedral angle between the tetrazole and benzene rings is  $17.2(2)^\circ$ . In the crystal,  $\text{C}-\text{H}\cdots\text{N}$  interactions link the molecules into a flattened helical chain along the  $b$  axis.

## Related literature

For related structures, see: Baek *et al.* (2012); Matsunaga *et al.* (1999); Lyakhov *et al.* (2000, 2001). For the synthesis, see: Su *et al.* (2006).



## Experimental

## Crystal data

$\text{C}_7\text{H}_4\text{Cl}_2\text{N}_4$   
 $M_r = 215.04$   
 Monoclinic,  $P2_1/c$   
 $a = 3.8362(2)$  Å

$b = 9.0524(3)$  Å  
 $c = 24.8876(11)$  Å  
 $\beta = 91.956(4)^\circ$   
 $V = 863.76(7)$  Å<sup>3</sup>

$Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.70$  mm<sup>-1</sup>

$T = 293$  K  
 $0.3 \times 0.2 \times 0.2$  mm

## Data collection

Oxford Diffraction Xcalibur  
 Sapphire3 diffractometer  
 Absorption correction: multi-scan  
 (*CrysAlis PRO*; Oxford  
 Diffraction, 2010)  
 $T_{\min} = 0.699$ ,  $T_{\max} = 0.869$

16772 measured reflections  
 1692 independent reflections  
 1451 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.048$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.057$   
 $wR(F^2) = 0.114$   
 $S = 1.17$   
 1692 reflections

118 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.31$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.25$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C1}-\text{H1}\cdots\text{N2}^i$	0.93	2.61	3.423 (5)	147
$\text{C7}-\text{H7}\cdots\text{N1}^i$	0.93	2.53	3.424 (5)	161

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

YTJ is grateful for the support provided by the second stage of BK21 Program. RK thanks the DST, New Delhi, India, for the X-ray data collection facility.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS5049).

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**supplementary materials**

*Acta Cryst.* (2012). E68, o433 [ doi:10.1107/S1600536812001225 ]

## 1-(3,5-Dichlorophenyl)-1*H*-1,2,3,4-tetrazole

R. G. Kalkhambkar, D. Gayathri, V. K. Gupta, R. Kant and Y. T. Jeong

### Comment

In continuation of our work on tetrazole based heterocycles, we are here in reporting the crystal structure of the title compound.

Bond lengths and angles are comparable with the similar crystal structures (Baek *et al.*, 2012; Lyakhov *et al.*, 2000, 2001; Matsunaga *et al.*, 1999). The tetrazole and phenyl rings are planar, with a maximum out-of-plane deviation of 0.007 (2) Å for each ring (r.m.s. deviation for each ring = 0.005 Å). The two rings are not coplanar with a dihedral angle being 17.2 (2)°. Chlorine atoms Cl1 and Cl2 deviate -0.002 (4) and 0.057 (5) Å, respectively, from the benzene plane. The crystal packing is stabilized by C—H···N intermolecular interactions, wherein atoms C1 and C7 act as a donor to N2 and N1, respectively, generating C(4) and C(6) chains along [010].

### Experimental

The title compound was synthesized from the known procedure reported by Su *et al.* (2006). Fine white diffraction quality crystals were obtained from the slow evaporation of its solution in ethanol.

### Refinement

All H atoms were refined using a riding model, with C—H = 0.93 Å, and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

### Figures

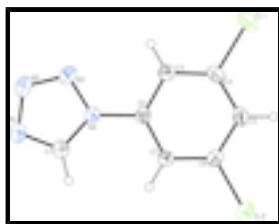


Fig. 1. The molecular structure of the title compound, showing 30% probability displacement ellipsoids.

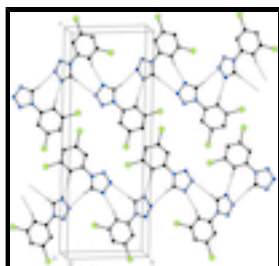


Fig. 2. The molecular packing of the title compound, showing intermolecular interactions. For clarity, hydrogen atoms not involved in hydrogen bonding have been omitted.

## 1-(3,5-Dichlorophenyl)-1H-1,2,3,4-tetrazole

### Crystal data

$C_7H_4Cl_2N_4$	$F(000) = 432$
$M_r = 215.04$	$D_x = 1.654 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Hall symbol: -P 2ybc	Cell parameters from 7140 reflections
$a = 3.8362 (2) \text{ \AA}$	$\theta = 4.0\text{--}29.0^\circ$
$b = 9.0524 (3) \text{ \AA}$	$\mu = 0.70 \text{ mm}^{-1}$
$c = 24.8876 (11) \text{ \AA}$	$T = 293 \text{ K}$
$\beta = 91.956 (4)^\circ$	Block, white
$V = 863.76 (7) \text{ \AA}^3$	$0.3 \times 0.2 \times 0.2 \text{ mm}$
$Z = 4$	

### Data collection

Oxford Diffraction Xcalibur Sapphire3 diffractometer	1692 independent reflections
Radiation source: fine-focus sealed tube graphite	1451 reflections with $I > 2\sigma(I)$
Detector resolution: 16.1049 pixels $\text{mm}^{-1}$	$R_{\text{int}} = 0.048$
$\omega$ scans	$\theta_{\text{max}} = 26.0^\circ$ , $\theta_{\text{min}} = 4.0^\circ$
Absorption correction: multi-scan ( <i>CrysAlis PRO</i> ; Oxford Diffraction, 2010)	$h = -4 \rightarrow 4$
$T_{\text{min}} = 0.699$ , $T_{\text{max}} = 0.869$	$k = -11 \rightarrow 11$
16772 measured reflections	$l = -30 \rightarrow 30$

### Refinement

Refinement on $F^2$	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.057$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.114$	H-atom parameters constrained
$S = 1.17$	$w = 1/[\sigma^2(F_o^2) + (0.0229P)^2 + 1.3257P]$
1692 reflections	where $P = (F_o^2 + 2F_c^2)/3$
118 parameters	$(\Delta/\sigma)_{\text{max}} < 0.001$
0 restraints	$\Delta\rho_{\text{max}} = 0.31 \text{ e \AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.25 \text{ e \AA}^{-3}$

### 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  $F^2 > \sigma(F^2)$  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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.8151 (11)	0.8952 (4)	0.22313 (15)	0.0569 (10)
H1	0.7634	0.8155	0.2450	0.068*
C2	0.5993 (8)	0.7942 (3)	0.13392 (12)	0.0332 (7)
C3	0.4810 (8)	0.8412 (4)	0.08358 (13)	0.0389 (7)
H3	0.4966	0.9397	0.0734	0.047*
C4	0.3391 (8)	0.7360 (4)	0.04919 (12)	0.0410 (8)
C5	0.3089 (8)	0.5895 (4)	0.06386 (13)	0.0405 (8)
H5	0.2125	0.5202	0.0401	0.049*
C6	0.4258 (8)	0.5491 (3)	0.11477 (13)	0.0378 (7)
C7	0.5739 (8)	0.6494 (3)	0.15071 (12)	0.0348 (7)
H7	0.6533	0.6204	0.1848	0.042*
N1	0.9600 (10)	1.0175 (4)	0.23973 (13)	0.0619 (9)
N2	0.9905 (10)	1.1003 (4)	0.19516 (15)	0.0682 (10)
N3	0.8690 (10)	1.0311 (3)	0.15319 (13)	0.0655 (10)
N4	0.7517 (7)	0.9004 (3)	0.17044 (11)	0.0379 (6)
Cl1	0.1904 (3)	0.78829 (13)	-0.01453 (4)	0.0645 (3)
Cl2	0.3786 (3)	0.36798 (10)	0.13489 (4)	0.0639 (3)

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.084 (3)	0.043 (2)	0.042 (2)	-0.014 (2)	-0.0130 (19)	0.0013 (16)
C2	0.0334 (16)	0.0344 (16)	0.0319 (16)	-0.0010 (13)	0.0023 (12)	-0.0025 (13)
C3	0.0421 (18)	0.0371 (18)	0.0375 (17)	-0.0027 (14)	-0.0005 (14)	0.0056 (14)
C4	0.0377 (17)	0.054 (2)	0.0309 (16)	-0.0017 (15)	-0.0021 (13)	0.0045 (15)
C5	0.0388 (18)	0.0460 (19)	0.0367 (17)	-0.0075 (15)	-0.0016 (14)	-0.0061 (15)
C6	0.0403 (17)	0.0319 (16)	0.0414 (18)	-0.0016 (14)	0.0022 (14)	-0.0008 (14)
C7	0.0375 (17)	0.0351 (17)	0.0317 (16)	-0.0022 (13)	-0.0007 (13)	0.0018 (13)
N1	0.087 (3)	0.0454 (18)	0.052 (2)	-0.0120 (18)	-0.0179 (17)	-0.0070 (15)
N2	0.096 (3)	0.0420 (18)	0.065 (2)	-0.0217 (18)	-0.015 (2)	-0.0050 (17)
N3	0.103 (3)	0.0397 (17)	0.053 (2)	-0.0251 (18)	-0.0099 (19)	0.0065 (15)
N4	0.0451 (15)	0.0307 (14)	0.0375 (14)	-0.0040 (12)	-0.0038 (12)	-0.0002 (11)
Cl1	0.0754 (7)	0.0796 (7)	0.0374 (5)	-0.0070 (6)	-0.0160 (4)	0.0084 (5)
Cl2	0.0968 (8)	0.0353 (5)	0.0589 (6)	-0.0147 (5)	-0.0059 (5)	0.0006 (4)

*Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )*

C1—N1	1.300 (5)	C4—Cl1	1.733 (3)
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## supplementary materials

C1—N4	1.326 (4)	C5—C6	1.379 (4)
C1—H1	0.9300	C5—H5	0.9300
C2—C7	1.381 (4)	C6—C7	1.383 (4)
C2—C3	1.384 (4)	C6—C12	1.726 (3)
C2—N4	1.434 (4)	C7—H7	0.9300
C3—C4	1.380 (4)	N1—N2	1.347 (5)
C3—H3	0.9300	N2—N3	1.291 (4)
C4—C5	1.382 (5)	N3—N4	1.342 (4)
N1—C1—N4	110.3 (3)	C4—C5—H5	121.0
N1—C1—H1	124.9	C5—C6—C7	122.3 (3)
N4—C1—H1	124.9	C5—C6—C12	119.0 (2)
C7—C2—C3	122.7 (3)	C7—C6—C12	118.7 (2)
C7—C2—N4	118.4 (3)	C2—C7—C6	117.3 (3)
C3—C2—N4	118.8 (3)	C2—C7—H7	121.3
C4—C3—C2	117.4 (3)	C6—C7—H7	121.3
C4—C3—H3	121.3	C1—N1—N2	105.1 (3)
C2—C3—H3	121.3	N3—N2—N1	110.9 (3)
C3—C4—C5	122.2 (3)	N2—N3—N4	106.5 (3)
C3—C4—C11	119.3 (3)	C1—N4—N3	107.2 (3)
C5—C4—C11	118.4 (3)	C1—N4—C2	131.3 (3)
C6—C5—C4	118.0 (3)	N3—N4—C2	121.5 (3)
C6—C5—H5	121.0		
C7—C2—C3—C4	-1.3 (5)	N4—C1—N1—N2	-0.8 (5)
N4—C2—C3—C4	179.3 (3)	C1—N1—N2—N3	0.0 (5)
C2—C3—C4—C5	1.0 (5)	N1—N2—N3—N4	0.7 (5)
C2—C3—C4—C11	-179.5 (2)	N1—C1—N4—N3	1.2 (5)
C3—C4—C5—C6	0.0 (5)	N1—C1—N4—C2	179.6 (3)
C11—C4—C5—C6	-179.6 (2)	N2—N3—N4—C1	-1.2 (4)
C4—C5—C6—C7	-0.8 (5)	N2—N3—N4—C2	-179.7 (3)
C4—C5—C6—C12	178.0 (3)	C7—C2—N4—C1	-16.1 (5)
C3—C2—C7—C6	0.6 (5)	C3—C2—N4—C1	163.4 (4)
N4—C2—C7—C6	180.0 (3)	C7—C2—N4—N3	162.1 (3)
C5—C6—C7—C2	0.5 (5)	C3—C2—N4—N3	-18.4 (5)
C12—C6—C7—C2	-178.3 (2)		

### Hydrogen-bond geometry ( $\text{\AA}$ , $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C1—H1 $\cdots$ N2 <sup>i</sup>	0.93	2.61	3.423 (5)	147
C7—H7 $\cdots$ N1 <sup>i</sup>	0.93	2.53	3.424 (5)	161

Symmetry codes: (i)  $-x+2, y-1/2, -z+1/2$ .

Fig. 1

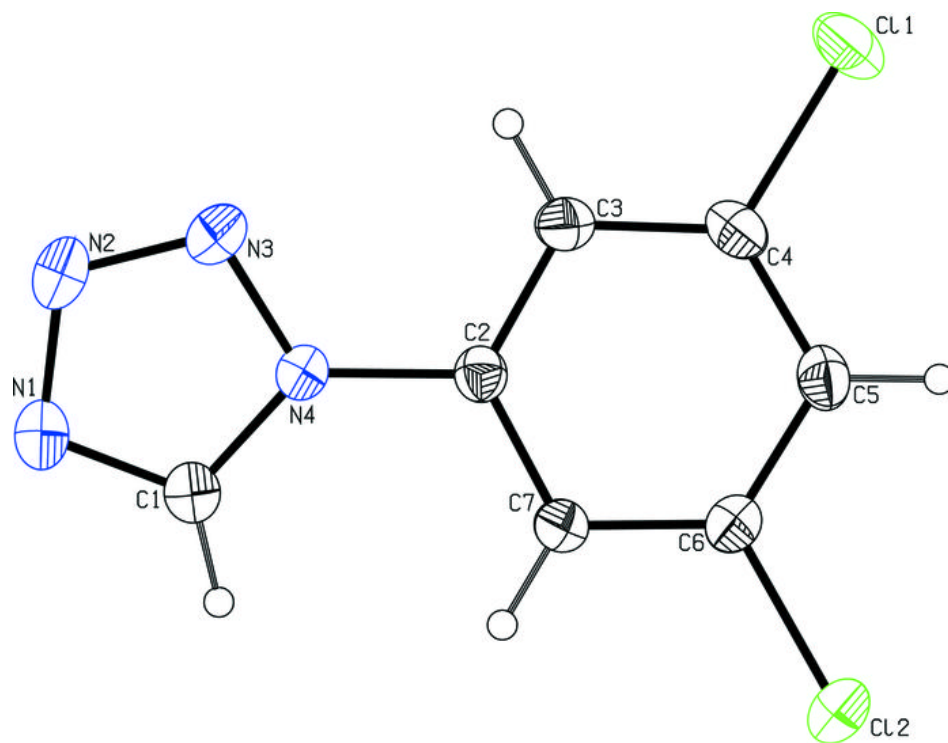


Fig. 2

