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4-[2-(4-Chlorophenyl)-3-methylbutanamido]-3-*p*-tolyl-1*H*-1,2,4-triazole-5(4*H*)-thione dimethylformamide solvate

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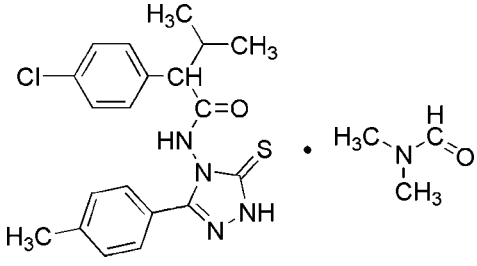
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.059; wR factor = 0.184; data-to-parameter ratio = 17.5.

In the title compound, $C_{20}H_{21}ClN_4OS\cdot C_3H_7NO$, the molecules are linked to each other through an N—H···O hydrogen bond to form chains to which the dimethylformamide solvent molecules are attached *via* a second N—H···O interaction. Bond lengths and angles are unexceptional.

Related literature

For related literature, see: Cansiz *et al.* (2001); Kane *et al.* (1988); Reid & Heindel (1976); Sughen & Yoloye (1978); Zhang *et al.* (1990).



Experimental

Crystal data

$C_{20}H_{21}ClN_4OS\cdot C_3H_7NO$
M_r = 474.01
Monoclinic, $P2_1/c$
a = 10.235 (4) Å
b = 26.654 (12) Å
c = 9.581 (4) Å
β = 93.963 (6)°
V = 2607.6 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.25 mm^{-1}
T = 298 (2) K
0.30 × 0.15 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.918, T_{max} = 0.975
11679 measured reflections
5098 independent reflections
2828 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.184
S = 0.96
5098 reflections
292 parameters
44 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2B···O2^{i}	0.86	1.86	2.694 (4)	164
N4—H4A···O1^{ii}	0.86	1.97	2.824 (3)	170

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2045).

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supplementary materials

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4-[2-(4-Chlorophenyl)-3-methylbutanamido]-3-*p*-tolyl-1*H*-1,2,4-triazole-5(4*H*)-thione dimethylformamide solvate

S.-J. Xue, A. Chai, Z.-J. Cai, C.-S. Xiang and W.-D. Bian

Comment

Substituted 1,2,4-triazoles have received much attention on account of their important pharmacological activites, such as antiviral, analgesic, antimicrobial, antidepressant and antifungal effect (Sughen & Yoloye, 1978; Cansiz *et al.*,2001; Kane *et al.*, 1988). Based on the excellent properties of substituted 1,2,4-triazole, we attempted to incorporate 2-(4-chlorophenyl)-3-methylbutanoic acid into the triazole ring system, hoping to find for a novel triazole compound with higher bioactivity. We report here the synthesis and crystal structure of the title compound (I), obtained during this process (Scheme 1).

There are three aromatic rings in the structure, namely a triazole (N1→ N3/C12/C13), a methylbenzene (C14→ C20), and a chlorobenzene (C1→ C6) rings, (Fig 1). The *p*-methylbenzene and 4-chlorobenzene planes make a dihedral angle of 38.2 (5)°, while the 1,2,4-triazole ring forms dihedral angles of 31.5 (0)° and 68.3 (1)° with the *p*-methylbenzene and 4-chlorobenzene rings, respectively. Bonds and angles in (I) are unexceptional.

The molecules link to each other into chains through a N—H···O hydrogen bond; in turn, the dimethylformamide solvato molecules are attached to these one-dimensional structures *via* a second N—H···O interaction (Table 2 and Figures 1 and 2).

Experimental

3-aryl-4-amino −5-mercapto-1,2,4-triazole was prepared by the literature method (Zhang *et al.*, 1990; Reid & Heindel, 1976). 2-(4-chlorophenyl)-3-methylbutanoic acid (0.01 mol) and sulfuric chloride (10 ml) were placed in a dried round-bottomed flask containing a magnetic stirrer bar and stirred at 75°C for 1.5 h. Then the excessive sulfuric chloride was removed under reduced pressure, and the residue left to cool to room temperature to obtain the 2-(4-chlorophenyl)-3-methylbutanoyl chloride. Then 3-aryl-4-amino-5-mercapto-1,2,4-triazole (0.008 mol) and 20 ml anhydrous acetonitrile were added. The reaction mixture was stirred at refluxed temperature and monitored by TLC. After refluxing for 3 h, the undisolved by-products were removed by filtration immediately and the product (I) precipitated from the filtrate when the solution was cooled to room temperature. It was further purified by recrystallization in ethanol. Crystals suitable for single-crystal X-ray diffraction were obtained by cooling the hot solution of *N*,*N*'-dimethylformamide. ^{1}H NMR (DMSO-d$_6$, 400 MHz): 11.30 (s, 1H, NH), 7.92–7.00 (m, 8H, Ph—H), 3.76 (d, 1H, —C—H), 3.00 (s, 1H, S—H), 2.52 (m, 1H, —C—H), 2.35 (s, 3H, Ph—CH$_3$), 1.10 (d, 6H, —CH$_3$); Analysis calculated for $C_{20}H_{21}ClN_4OS$: C 59.91, H 5.28, N 13.97%; found: C 59.97, H 5.25, N 14.00%.

Refinement

The H atoms were positioned geometrically (C—H = 0.93, 0.96 or 0.98 A ° and N—H = 0.86 A °) and refined using the riding-model approximation, with U_{iso}(H) = 1.2Ueq(C, *N*).

Figures

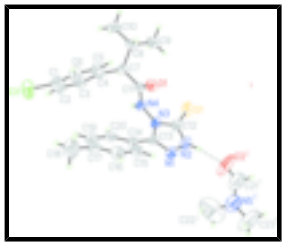


Figure 1. The molecular structure of (I), showing the atom-numbering scheme. The hydrogen bond linking the molecule and the solvate is shown in dashed line. Displacement ellipsoids drawn at a 30% level. Symmetry code (i): $x,y,z+1$

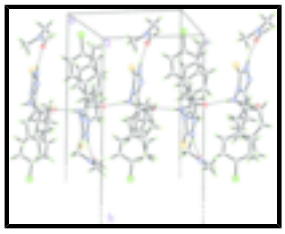
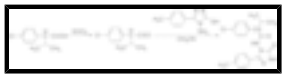


Figure 2. View of the molecular chain in (I). Hydrogen bonds are shown as dashed lines.



4-[2-(4-Chlorophenyl)-3-methylbutanamido]-3-*p*-tolyl-1*H*-1,2,4- triazole-5(4*H*)-thione dimethylformamide solvate

Crystal data

$C_{20}H_{21}ClN_4OS\cdot C_3H_7NO$	F_{000} = 1000
M_r = 474.01	D_x = 1.207 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 846 reflections
a = 10.235 (4) Å	θ = 2.3–22.5º
b = 26.654 (12) Å	μ = 0.25 mm^{-1}
c = 9.581 (4) Å	T = 298 (2) K
β = 93.963 (6)º	T = 298 (2) K, colourless
V = 2607.6 (19) Å^3	0.30 × 0.15 × 0.10 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	5098 independent reflections
Radiation source: fine-focus sealed tube	2828 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.043
T = 298(2) K	θ_{max} = 26.0º
phi and ω scans	θ_{min} = 1.5º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	h = −12→12
T_{min} = 0.918, T_{max} = 0.975	k = −32→28
11679 measured reflections	l = −11→11

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.059$	H-atom parameters constrained
$wR(F^2) = 0.184$	$w = 1/[\sigma^2(F_o^2) + (0.1043P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.96$	$(\Delta/\sigma)_{max} < 0.001$
5098 reflections	$\Delta\rho_{max} = 0.35$ e Å^{-3}
292 parameters	$\Delta\rho_{min} = -0.26$ e Å^{-3}
44 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 $F^2 > 2\text{sigma}(F^2)$ 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.16930 (14)	−0.00080 (4)	0.83559 (14)	0.1301 (5)
S1	0.11276 (10)	0.38390 (3)	0.82591 (9)	0.0871 (3)
N1	0.4180 (2)	0.31509 (10)	1.0000 (3)	0.0740 (7)
N2	0.3445 (3)	0.35624 (10)	0.9613 (3)	0.0757 (7)
H2B	0.3685	0.3863	0.9830	0.091*
N3	0.2390 (2)	0.29481 (8)	0.8760 (2)	0.0573 (6)
N4	0.1380 (2)	0.26553 (8)	0.8176 (2)	0.0538 (5)
H4A	0.1274	0.2620	0.7283	0.065*
O1	0.07115 (17)	0.24620 (7)	1.02859 (16)	0.0613 (5)
C1	0.1062 (3)	0.06002 (11)	0.8322 (4)	0.0793 (9)
C2	0.0941 (3)	0.08607 (12)	0.7078 (3)	0.0765 (8)
H2A	0.1195	0.0715	0.6257	0.092*
C3	0.0440 (3)	0.13405 (11)	0.7068 (3)	0.0634 (7)
H3A	0.0361	0.1518	0.6230	0.076*
C4	0.0052 (2)	0.15647 (10)	0.8272 (3)	0.0532 (6)
C5	0.0201 (3)	0.12912 (11)	0.9516 (3)	0.0689 (8)
H5A	−0.0035	0.1437	1.0345	0.083*

C6	0.0690 (3)	0.08105 (12)	0.9537 (3)	0.0817 (9)
H6A	0.0767	0.0630	1.0369	0.098*
C7	−0.0459 (2)	0.21000 (10)	0.8247 (2)	0.0516 (6)
H7A	−0.0541	0.2210	0.7269	0.062*
C8	−0.1804 (3)	0.21674 (12)	0.8848 (3)	0.0694 (8)
H8A	−0.1725	0.2071	0.9838	0.083*
C9	−0.2240 (3)	0.27065 (14)	0.8745 (4)	0.0927 (11)
H9A	−0.3071	0.2741	0.9141	0.139*
H9B	−0.2321	0.2806	0.7780	0.139*
H9C	−0.1605	0.2916	0.9248	0.139*
C10	−0.2807 (3)	0.18231 (16)	0.8079 (5)	0.1045 (13)
H10A	−0.3642	0.1864	0.8465	0.157*
H10B	−0.2527	0.1481	0.8186	0.157*
H10C	−0.2883	0.1909	0.7104	0.157*
C11	0.0567 (2)	0.24256 (9)	0.9014 (2)	0.0474 (6)
C12	0.2323 (3)	0.34601 (11)	0.8871 (3)	0.0642 (7)
C13	0.3519 (2)	0.27690 (10)	0.9485 (3)	0.0580 (7)
C14	0.3873 (2)	0.22500 (11)	0.9720 (3)	0.0599 (7)
C15	0.4576 (3)	0.21229 (13)	1.0973 (3)	0.0738 (8)
H15A	0.4821	0.2373	1.1615	0.089*
C16	0.4902 (3)	0.16410 (14)	1.1260 (4)	0.0909 (10)
H16A	0.5358	0.1565	1.2107	0.109*
C17	0.4573 (4)	0.12548 (14)	1.0319 (5)	0.0932 (11)
C18	0.4923 (6)	0.07157 (18)	1.0685 (7)	0.161 (2)
H18A	0.4611	0.0500	0.9933	0.241*
H18B	0.4524	0.0622	1.1524	0.241*
H18C	0.5857	0.0684	1.0830	0.241*
C19	0.3902 (3)	0.13830 (13)	0.9060 (4)	0.0860 (10)
H19A	0.3682	0.1133	0.8409	0.103*
C20	0.3556 (3)	0.18687 (11)	0.8756 (3)	0.0684 (8)
H20A	0.3109	0.1945	0.7905	0.082*
C21	0.5479 (7)	0.4571 (2)	0.1282 (8)	0.166 (2)
H21A	0.5274	0.4745	0.2080	0.199*
C22	0.7078 (11)	0.4277 (6)	0.0050 (10)	0.317 (6)
H22A	0.6383	0.4283	−0.0676	0.476*
H22B	0.7242	0.3937	0.0344	0.476*
H22C	0.7857	0.4416	−0.0298	0.476*
C23	0.7667 (9)	0.4766 (3)	0.2044 (15)	0.319 (6)
H23A	0.7278	0.5029	0.2562	0.479*
H23B	0.8348	0.4905	0.1521	0.479*
H23C	0.8031	0.4517	0.2681	0.479*
N5	0.6730 (5)	0.45505 (15)	0.1142 (6)	0.1469 (17)
O2	0.4539 (5)	0.44186 (13)	0.0628 (6)	0.209 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.1782 (12)	0.0764 (7)	0.1362 (10)	0.0280 (6)	0.0133 (8)	0.0057 (6)

S1	0.1223 (8)	0.0741 (5)	0.0620 (5)	0.0057 (5)	−0.0142 (5)	0.0044 (4)
N1	0.0710 (15)	0.0752 (17)	0.0742 (17)	−0.0165 (13)	−0.0059 (13)	−0.0077 (13)
N2	0.0882 (18)	0.0666 (16)	0.0709 (16)	−0.0202 (14)	−0.0050 (14)	−0.0068 (13)
N3	0.0638 (14)	0.0640 (14)	0.0435 (12)	−0.0132 (11)	−0.0007 (10)	−0.0030 (10)
N4	0.0629 (13)	0.0659 (13)	0.0317 (10)	−0.0124 (10)	−0.0016 (9)	−0.0028 (9)
O1	0.0723 (12)	0.0795 (12)	0.0319 (9)	0.0013 (9)	0.0020 (8)	−0.0017 (8)
C1	0.091 (2)	0.0603 (18)	0.086 (2)	−0.0022 (15)	0.0001 (18)	−0.0009 (17)
C2	0.091 (2)	0.076 (2)	0.064 (2)	−0.0011 (17)	0.0115 (16)	−0.0098 (16)
C3	0.0729 (18)	0.0675 (18)	0.0500 (16)	−0.0069 (14)	0.0044 (13)	−0.0027 (13)
C4	0.0482 (14)	0.0645 (16)	0.0466 (15)	−0.0098 (12)	0.0015 (11)	0.0006 (12)
C5	0.083 (2)	0.0725 (19)	0.0516 (17)	−0.0048 (15)	0.0051 (14)	0.0009 (14)
C6	0.105 (2)	0.075 (2)	0.065 (2)	−0.0041 (18)	0.0004 (17)	0.0130 (16)
C7	0.0475 (14)	0.0705 (16)	0.0365 (13)	−0.0047 (12)	0.0004 (10)	0.0020 (11)
C8	0.0513 (16)	0.100 (2)	0.0573 (17)	0.0042 (15)	0.0107 (13)	0.0022 (15)
C9	0.067 (2)	0.114 (3)	0.097 (3)	0.0212 (19)	0.0097 (18)	−0.004 (2)
C10	0.0508 (18)	0.132 (3)	0.130 (3)	−0.0175 (19)	0.007 (2)	−0.009 (2)
C11	0.0509 (14)	0.0570 (14)	0.0342 (13)	0.0073 (11)	0.0024 (10)	0.0011 (11)
C12	0.086 (2)	0.0645 (17)	0.0422 (14)	−0.0117 (15)	0.0037 (13)	−0.0023 (12)
C13	0.0538 (15)	0.0719 (18)	0.0482 (15)	−0.0135 (14)	0.0035 (12)	−0.0069 (13)
C14	0.0496 (15)	0.0718 (18)	0.0585 (17)	−0.0064 (13)	0.0051 (12)	−0.0030 (14)
C15	0.0668 (19)	0.090 (2)	0.0641 (19)	0.0027 (16)	−0.0001 (15)	−0.0052 (16)
C16	0.091 (2)	0.093 (3)	0.088 (2)	0.010 (2)	−0.0011 (19)	0.013 (2)
C17	0.080 (2)	0.078 (2)	0.122 (3)	0.0071 (18)	0.010 (2)	0.012 (2)
C18	0.172 (5)	0.090 (3)	0.216 (6)	0.016 (3)	−0.016 (4)	0.017 (3)
C19	0.0636 (19)	0.074 (2)	0.119 (3)	−0.0026 (16)	0.0008 (19)	−0.017 (2)
C20	0.0490 (15)	0.077 (2)	0.079 (2)	−0.0031 (13)	0.0018 (14)	−0.0107 (16)
C21	0.164 (5)	0.124 (4)	0.201 (6)	−0.014 (4)	−0.055 (5)	−0.012 (4)
C22	0.317 (12)	0.489 (18)	0.146 (7)	0.141 (11)	0.015 (7)	0.023 (7)
C23	0.211 (7)	0.139 (5)	0.576 (17)	−0.011 (5)	−0.202 (10)	−0.043 (8)
N5	0.143 (4)	0.094 (3)	0.196 (5)	0.006 (3)	−0.047 (4)	0.011 (3)
O2	0.230 (4)	0.111 (3)	0.268 (5)	−0.069 (3)	−0.103 (4)	−0.015 (3)

Geometric parameters (Å, °)

Cl1—C1	1.744 (3)	C9—H9C	0.9600
S1—C12	1.662 (3)	C10—H10A	0.9600
N1—C13	1.301 (3)	C10—H10B	0.9600
N1—N2	1.367 (3)	C10—H10C	0.9600
N2—C12	1.336 (4)	C13—C14	1.443 (4)
N2—H2B	0.8600	C14—C20	1.396 (4)
N3—C12	1.371 (4)	C14—C15	1.397 (4)
N3—N4	1.382 (3)	C15—C16	1.351 (5)
N3—C13	1.391 (3)	C15—H15A	0.9300
N4—C11	1.343 (3)	C16—C17	1.394 (5)
N4—H4A	0.8600	C16—H16A	0.9300
O1—C11	1.221 (3)	C17—C19	1.389 (5)
C1—C6	1.370 (5)	C17—C18	1.516 (6)
C1—C2	1.378 (4)	C18—H18A	0.9600
C2—C3	1.378 (4)	C18—H18B	0.9600

C2—H2A	0.9300	C18—H18C	0.9600
C3—C4	1.382 (4)	C19—C20	1.368 (4)
C3—H3A	0.9300	C19—H19A	0.9300
C4—C5	1.397 (4)	C20—H20A	0.9300
C4—C7	1.519 (4)	C21—O2	1.183 (7)
C5—C6	1.375 (4)	C21—N5	1.298 (7)
C5—H5A	0.9300	C21—H21A	0.9300
C6—H6A	0.9300	C22—N5	1.343 (10)
C7—C11	1.514 (3)	C22—H22A	0.9600
C7—C8	1.539 (4)	C22—H22B	0.9600
C7—H7A	0.9800	C22—H22C	0.9600
C8—C9	1.506 (5)	C23—N5	1.373 (8)
C8—C10	1.528 (5)	C23—H23A	0.9600
C8—H8A	0.9800	C23—H23B	0.9600
C9—H9A	0.9600	C23—H23C	0.9600
C9—H9B	0.9600		
C13—N1—N2	105.2 (2)	O1—C11—N4	121.5 (2)
C12—N2—N1	114.7 (2)	O1—C11—C7	124.2 (2)
C12—N2—H2B	122.7	N4—C11—C7	114.1 (2)
N1—N2—H2B	122.7	N2—C12—N3	101.5 (2)
C12—N3—N4	123.6 (2)	N2—C12—S1	130.4 (2)
C12—N3—C13	110.3 (2)	N3—C12—S1	128.1 (2)
N4—N3—C13	125.5 (2)	N1—C13—N3	108.3 (2)
C11—N4—N3	119.50 (19)	N1—C13—C14	124.9 (3)
C11—N4—H4A	120.3	N3—C13—C14	126.7 (2)
N3—N4—H4A	120.3	C20—C14—C15	118.3 (3)
C6—C1—C2	121.0 (3)	C20—C14—C13	123.4 (3)
C6—C1—Cl1	119.3 (3)	C15—C14—C13	118.4 (3)
C2—C1—Cl1	119.7 (3)	C16—C15—C14	120.7 (3)
C1—C2—C3	119.0 (3)	C16—C15—H15A	119.6
C1—C2—H2A	120.5	C14—C15—H15A	119.6
C3—C2—H2A	120.5	C15—C16—C17	121.7 (4)
C2—C3—C4	121.6 (3)	C15—C16—H16A	119.2
C2—C3—H3A	119.2	C17—C16—H16A	119.2
C4—C3—H3A	119.2	C19—C17—C16	117.6 (3)
C3—C4—C5	117.8 (3)	C19—C17—C18	121.9 (4)
C3—C4—C7	120.8 (2)	C16—C17—C18	120.5 (4)
C5—C4—C7	121.4 (2)	C17—C18—H18A	109.5
C6—C5—C4	121.1 (3)	C17—C18—H18B	109.5
C6—C5—H5A	119.4	H18A—C18—H18B	109.5
C4—C5—H5A	119.4	C17—C18—H18C	109.5
C1—C6—C5	119.4 (3)	H18A—C18—H18C	109.5
C1—C6—H6A	120.3	H18B—C18—H18C	109.5
C5—C6—H6A	120.3	C20—C19—C17	121.5 (3)
C11—C7—C4	107.71 (19)	C20—C19—H19A	119.2
C11—C7—C8	111.1 (2)	C17—C19—H19A	119.2
C4—C7—C8	114.8 (2)	C19—C20—C14	120.2 (3)
C11—C7—H7A	107.7	C19—C20—H20A	119.9
C4—C7—H7A	107.7	C14—C20—H20A	119.9

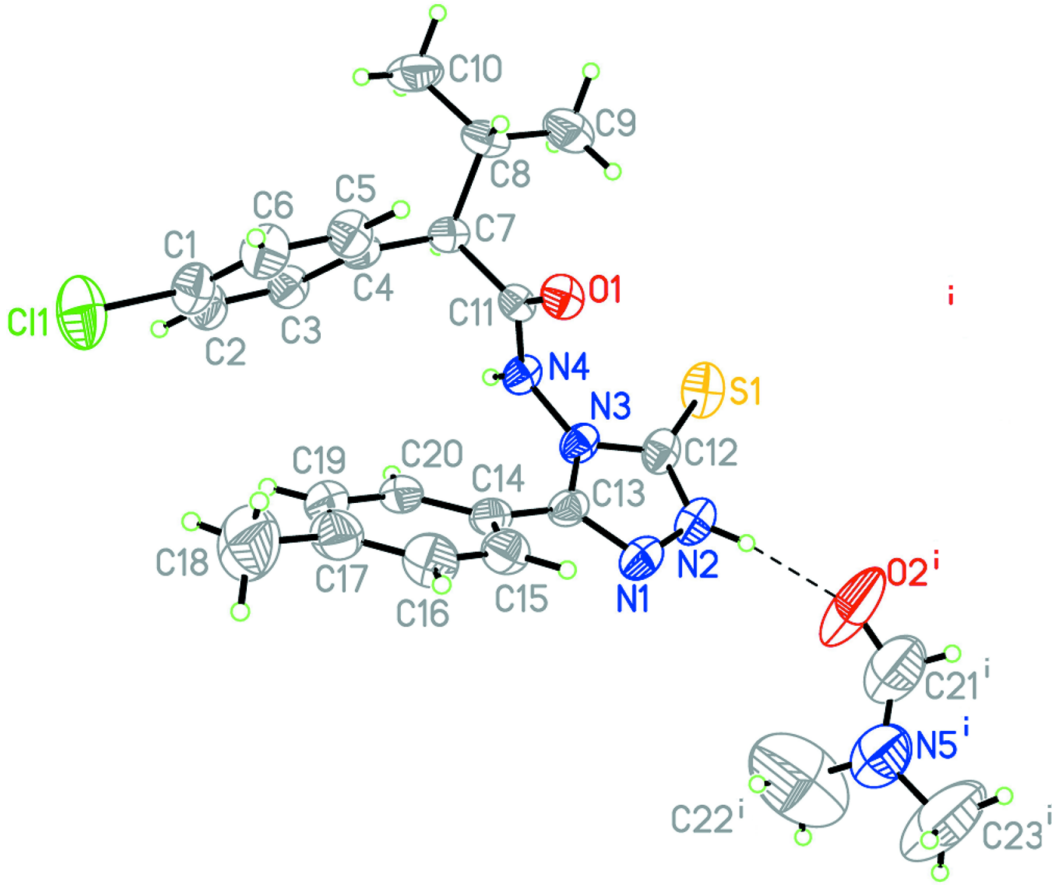
C8—C7—H7A	107.7	O2—C21—N5	134.6 (8)
C9—C8—C10	110.8 (3)	O2—C21—H21A	112.7
C9—C8—C7	110.8 (2)	N5—C21—H21A	112.7
C10—C8—C7	109.8 (2)	N5—C22—H22A	109.5
C9—C8—H8A	108.5	N5—C22—H22B	109.5
C10—C8—H8A	108.5	H22A—C22—H22B	109.5
C7—C8—H8A	108.5	N5—C22—H22C	109.5
C8—C9—H9A	109.5	H22A—C22—H22C	109.5
C8—C9—H9B	109.5	H22B—C22—H22C	109.5
H9A—C9—H9B	109.5	N5—C23—H23A	109.5
C8—C9—H9C	109.5	N5—C23—H23B	109.5
H9A—C9—H9C	109.5	H23A—C23—H23B	109.5
H9B—C9—H9C	109.5	N5—C23—H23C	109.5
C8—C10—H10A	109.5	H23A—C23—H23C	109.5
C8—C10—H10B	109.5	H23B—C23—H23C	109.5
H10A—C10—H10B	109.5	C21—N5—C22	114.8 (8)
C8—C10—H10C	109.5	C21—N5—C23	124.7 (8)
H10A—C10—H10C	109.5	C22—N5—C23	120.4 (9)
H10B—C10—H10C	109.5		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2B···O2^{i}	0.86	1.86	2.694 (4)	164
N4—H4A···O1^{ii}	0.86	1.97	2.824 (3)	170

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

Fig. 1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C9
C8
C5
C6
C7
C1
C4
Cl1
C2
C3
C11
O1
i
N4
S1
N3
C12
C19
C20
C14
C13
C18
C17
C16
C15
N1
N2
O2i
C21i
N5i
C22i
C23i

Fig. 2

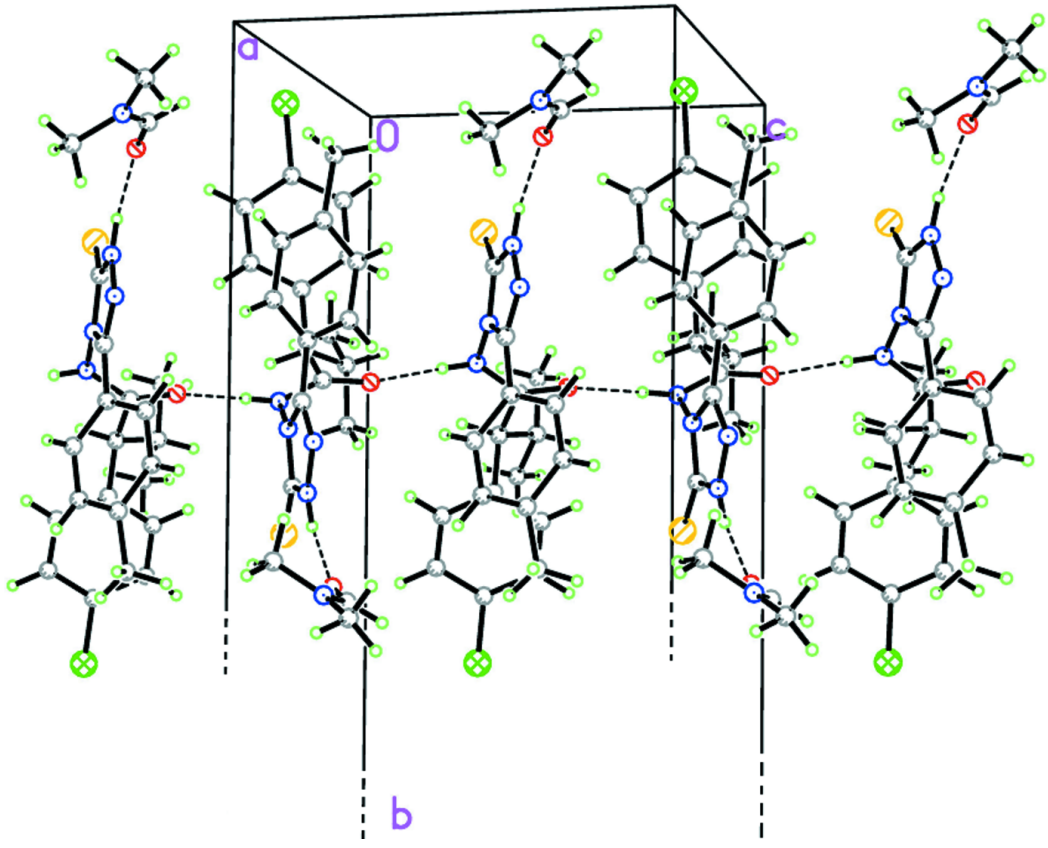
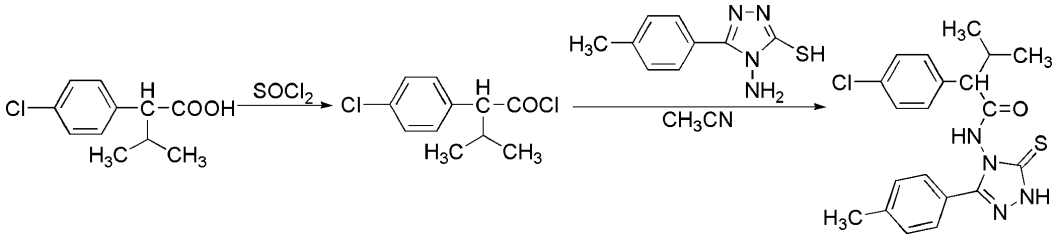


Fig. 3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NH2
CH3CN
Cl
H3C
CH3
CH
C=O
HN
N
S
NH
N
H3C