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1-(Acetonyl)-3-(2-thienylmethyl)-4-(4*H*-1,2,4-triazol-4-yl)-1*H*-1,2,4-triazol-5(4*H*)-one

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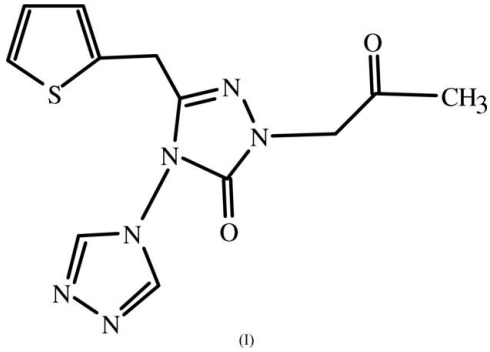
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.047; wR factor = 0.089; data-to-parameter ratio = 12.0.

In the title compound, $C_{12}H_{12}N_6O_2S$, the thiophene ring is disordered equally over two positions, corresponding to rotation of approximately 180° about the C—C single bond. The central triazole ring has substituents at the 1-, 3-, 4- and 5-positions. Intermolecular C—H···N and C—H···O interactions help to stabilize the structure.

Related literature

For related literature, see: Chai *et al.* (2003); Demirbaş *et al.* (2004); Er-Rahimini & Mornet (1992); Ichikawa *et al.* (2001); Jenkins *et al.* (1989); Kim *et al.* (2003); Nakib *et al.* (1994); Palmer & Parsons (1996); Puviarasan *et al.* (1999); Sancak *et al.* (2005); Shaikh *et al.* (2002); Tsuda *et al.* (2004); Ueda (2003); Vrábel *et al.* (2005); Yılmaz, Arslan, Kazak, Sancak & Er (2006); Çoruh, Kahveci, Şaşmaz, Ağar & Kim (2003); Çoruh, Kahveci, Şaşmaz, Ağar, Kim & Erdönmez (2003).



(I)

Experimental

Crystal data

$C_{12}H_{12}N_6O_2S$
M_r = 304.34
Monoclinic, $P2_1/c$
a = 5.8357 (8) Å
b = 32.084 (4) Å
c = 7.4958 (10) Å
β = 95.087 (3)°
V = 1397.9 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.25 mm^{-1}
T = 293 (2) K
0.37 × 0.30 × 0.13 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.685, T_{max} = 0.969
6559 measured reflections
2412 independent reflections
1214 reflections with $I > 2\sigma(I)$
R_{int} = 0.086

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.089
S = 0.82
2412 reflections
201 parameters
183 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2019).

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supplementary materials

Acta Cryst. (2007). E**63**, o2774-o2775 [**doi:10.1107/S1600536807020326**]

1-(Acetonyl)-3-(2-thienylmethyl)-4-(4*H*-1,2,4-triazol-4-yl)-1*H*-1,2,4-triazol-5(4*H*)-one

R. Ustabas, U. Çoruh, K. Sancak, E. Demirkan and E. M. Vázquez-López

Comment

In a continuing search for pharmacologically active, 1,2,4-triazol and 1,2,4 triazol-5-one compounds it was found that most azole fungicides have been developed for diseases of cereal crops; examples include fluconazole (Ichikawa *et al.*, 2001), ravuconazole(Ueda, 2003) and posaconazole (Kim *et al.*, 2003). The properties of 1,2,4-triazole derivatives have broad-spectrum biological effects, such as insecticidal (Tsuda *et al.*, 2004), herbicidal (Chai *et al.*, 2003), anticonvulsant (Er-Rahimini & Mornet, 1992), antitumour (Nakip *et al.*, 1994) and plant growth regulatory activities (Jenkins *et al.*, 1989). Di- or tri-substituted 1,2,4-triazole derivatives have also been reported to show antituberculotic and antimicrobial activities (Demirbaş *et al.*, 2004). Additionally, thermally stable polymers containing the 1, 2, 4-triazole moiety have been prepared (Shaikh *et al.*, 2002).

The title compound (I)(Fig.1) consists of a triazole ring with an acetonyl group substituted at N4, a disordered (2,5-thienyl methyl) group substituted at C2, a 1,2,4-triazole ring substituted at N1 and an oxo O atom at C5. The N1—C5 bond length, 1.396 (3) Å, agrees with reported values [1.390 (3)Å in $C_{13}H_{13}ClN_4O_2$ (Çoruh, Kahveci, Şaşmaz, Ağar, Kim & Erdönmez, 2003), 1.387 (3)Å in $C_{12}H_{11}ClN_4O_2$ (Çoruh, Kahveci, Şaşmaz, Ağar & Kim, 2003)]. In the 1,2,4-triazole ring the N12—N13 bond length, 1.404 (4) Å, agrees with reported values [1.403 (8)Å in $C_{19}H_{18}N_6O_2S$ (Sancak *et al.*, 2005)].

The presence of a substituent on N4 causes a lengthening of the N—N bond length [N3—N4= 1.390 (3) Å] with respect to the corresponding bonds in 5-(2-chlorophenyl)-4-phenyl-3,4-dihydro-2*H*-1,2,4-triazole-3-thione [N—N= 1.374 (2) Å; Puviarasan *et al.*, 1999] and in 4-methyl-1,2,4- triazole and 1-methyltetrazole [N—N= 1.344 (2) Å; Palmer & Parsons, 1996]. The S—C bond lengths [S21—C22= 1.681 (4)Å and S21—C25= 1.6807 Å] agree with values reported in the literature [S41—C44=1.676 (4)Å and S41—C41=1.689 (3)Å (Vrabel *et al.*, 2005), C14—S1=1.692Å and C11—S1=1.708Å (Yılmaz *et al.*, 2006)].

The thiophene ring is disordered over two positions, corresponding to rotation of approximately 180° about the single C21—C22 bond, with a major-minor ratio of about 50:50. Intermolecular hydrogen bonds are effective in stabilizing the crystal structure.

Experimental

5-(Thien-2-ylmethyl)4, 4'-bi-1, 2, 4-triazol-3(2*H*)-one (0.001 mol) was refluxed with sodium metal (0.001 mol) in absolute ethanol (50 ml) for 1 h. Chloro acetone (0.001 mol) was added and the solution refluxed for 8 h. The resulting solution was filtered and then evaporated under reduced pressure. The solid residue was crystallized from absolute ethanol-diethylether (1:4). (Yield: 52 %; m.p. 438-439 K).

Refinement

H atoms were placed in idealized positions and were constrained using riding models at distances ranging between 0.93-0.97Å with isotropic displacement parameters derived from their carrier atoms (U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C_{Me}).

Figures

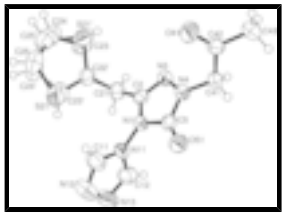


Fig. 1. An ORTEP drawing of (I), with the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

1-(Acetonyl)-3-(2-thienylmethyl)-4-(4*H*-1,2,4-triazol-4-yl)-1*H*- 1,2,4-triazol-5(4*H*)-one

Crystal data

$C_{12}H_{12}N_6O_2S$	F_{000} = 632
M_r = 304.34	D_x = 1.446 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 1214 reflections
a = 5.8357 (8) Å	θ = 2.5–25.3º
b = 32.084 (4) Å	μ = 0.25 mm^{-1}
c = 7.4958 (10) Å	T = 293 (2) K
β = 95.087 (3)º	Irregular, colorless
V = 1397.9 (3) Å^3	0.37 × 0.30 × 0.13 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	2412 independent reflections
Radiation source: fine-focus sealed tube	1214 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.086
T = 293(2) K	θ_{max} = 25.3º
φ and ω scans	θ_{min} = 2.5º
Absorption correction: multi-scan (SADABS; Bruker, 1997)	h = −6→7
T_{min} = 0.685, T_{max} = 0.969	k = −38→38
6559 measured reflections	l = −8→5

Refinement

Refinement on F^2	H-atom parameters constrained

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.047$

$wR(F^2) = 0.089$

$S = 0.82$

2412 reflections

201 parameters

183 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

$w = 1/[\sigma^2(F_o^2) + (0.028P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.17$ e Å^{-3}

$\Delta\rho_{min} = -0.17$ e Å^{-3}

Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0045 (8)

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.

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}	Occ. (<1)
C21	−0.1123 (5)	0.62882 (8)	0.4109 (4)	0.0508 (8)	
H21A	−0.2652	0.6397	0.4233	0.061*	
H21B	−0.1177	0.6134	0.2992	0.061*	
C22	0.0521 (5)	0.66449 (9)	0.4029 (4)	0.0505 (7)	0.50
C23	0.238 (2)	0.6635 (5)	0.313 (2)	0.0758 (7)	0.50
H23	0.2751	0.6408	0.2430	0.091*	0.50
C24	0.379 (3)	0.7009 (3)	0.332 (2)	0.0774 (13)	0.50
H24	0.5122	0.7057	0.2763	0.093*	0.50
C25	0.2859 (7)	0.72750 (11)	0.4445 (5)	0.0764 (12)	0.50
H25	0.3509	0.7531	0.4787	0.092*	0.50
S21	0.0395 (7)	0.70954 (11)	0.5162 (5)	0.0742 (7)	0.50
C22'	0.0521 (5)	0.66449 (9)	0.4029 (4)	0.0505 (7)	0.50
C23'	0.021 (3)	0.7032 (4)	0.4704 (18)	0.0742 (7)	0.50
H23'	−0.1058	0.7117	0.5278	0.089*	0.50
C24'	0.2230 (14)	0.7298 (3)	0.4377 (10)	0.0764 (12)	0.50
H24'	0.2445	0.7570	0.4781	0.092*	0.50
C25'	0.366 (3)	0.7094 (3)	0.344 (2)	0.0774 (13)	0.50
H25'	0.5009	0.7210	0.3092	0.093*	0.50

S21'	0.2842 (6)	0.66048 (14)	0.2919 (6)	0.0758 (7)	0.50
N1	−0.0889 (3)	0.60701 (6)	0.7383 (3)	0.0403 (6)	
C2	−0.0471 (4)	0.59995 (8)	0.5620 (4)	0.0399 (7)	
N3	0.0634 (4)	0.56527 (7)	0.5507 (3)	0.0457 (6)	
N4	0.0926 (3)	0.54966 (6)	0.7243 (3)	0.0419 (6)	
C5	−0.0098 (4)	0.57328 (8)	0.8443 (4)	0.0421 (7)	
O51	−0.0271 (3)	0.56817 (5)	1.0029 (3)	0.0559 (6)	
N11	−0.2326 (4)	0.63674 (6)	0.7998 (3)	0.0439 (6)	
O41	0.5537 (3)	0.53282 (6)	0.7185 (3)	0.0744 (7)	
C41	0.1784 (4)	0.50814 (7)	0.7550 (4)	0.0456 (7)	
H41A	0.0980	0.4897	0.6682	0.055*	
H41B	0.1426	0.4993	0.8730	0.055*	
C42	0.4318 (5)	0.50339 (9)	0.7430 (3)	0.0440 (7)	
C43	0.5203 (5)	0.45964 (8)	0.7612 (4)	0.0584 (8)	
H43A	0.6821	0.4601	0.7981	0.088*	
H43B	0.4949	0.4456	0.6481	0.088*	
H43C	0.4407	0.4451	0.8492	0.088*	
N12	−0.3510 (6)	0.68921 (9)	0.9474 (4)	0.0846 (9)	
N13	−0.5427 (5)	0.66589 (10)	0.8810 (4)	0.0817 (9)	
C12	−0.4651 (5)	0.63472 (10)	0.7955 (4)	0.0630 (9)	
H12	−0.5556	0.6139	0.7391	0.076*	
C11	−0.1712 (6)	0.67082 (9)	0.8970 (4)	0.0649 (9)	
H11	−0.0206	0.6798	0.9241	0.078*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C21	0.0548 (19)	0.0479 (18)	0.049 (2)	0.0007 (15)	0.0017 (16)	0.0037 (15)
C22	0.0550 (17)	0.0433 (15)	0.0531 (18)	0.0029 (13)	0.0045 (15)	0.0094 (14)
C23	0.0557 (16)	0.0810 (11)	0.0934 (14)	0.0008 (12)	0.0219 (11)	0.0207 (10)
C24	0.066 (2)	0.074 (3)	0.092 (3)	−0.010 (2)	0.0082 (18)	0.024 (2)
C25	0.085 (3)	0.059 (2)	0.085 (2)	−0.016 (2)	0.002 (2)	0.0139 (18)
S21	0.0963 (14)	0.0515 (13)	0.078 (2)	−0.0098 (11)	0.0229 (14)	−0.0079 (11)
C22'	0.0550 (17)	0.0433 (15)	0.0531 (18)	0.0029 (13)	0.0045 (15)	0.0094 (14)
C23'	0.0963 (14)	0.0515 (13)	0.078 (2)	−0.0098 (11)	0.0229 (14)	−0.0079 (11)
C24'	0.085 (3)	0.059 (2)	0.085 (2)	−0.016 (2)	0.002 (2)	0.0139 (18)
C25'	0.066 (2)	0.074 (3)	0.092 (3)	−0.010 (2)	0.0082 (18)	0.024 (2)
S21'	0.0557 (16)	0.0810 (11)	0.0934 (14)	0.0008 (12)	0.0219 (11)	0.0207 (10)
N1	0.0394 (14)	0.0349 (13)	0.0476 (16)	0.0072 (11)	0.0093 (12)	0.0006 (12)
C2	0.0347 (17)	0.0408 (18)	0.0445 (19)	−0.0041 (14)	0.0048 (14)	−0.0011 (15)
N3	0.0496 (16)	0.0409 (14)	0.0481 (16)	0.0039 (11)	0.0119 (12)	0.0005 (12)
N4	0.0441 (15)	0.0343 (13)	0.0481 (16)	0.0058 (11)	0.0087 (12)	0.0043 (12)
C5	0.0342 (18)	0.0373 (17)	0.055 (2)	−0.0024 (13)	0.0060 (16)	0.0045 (17)
O51	0.0665 (15)	0.0568 (13)	0.0458 (13)	0.0074 (10)	0.0124 (11)	0.0097 (11)
N11	0.0423 (15)	0.0369 (13)	0.0535 (16)	0.0049 (12)	0.0103 (12)	−0.0045 (12)
O41	0.0484 (14)	0.0548 (13)	0.121 (2)	−0.0130 (11)	0.0126 (13)	−0.0001 (13)
C41	0.0428 (18)	0.0358 (16)	0.059 (2)	0.0027 (13)	0.0107 (15)	0.0047 (14)
C42	0.0396 (17)	0.0449 (18)	0.0478 (19)	0.0000 (15)	0.0052 (15)	−0.0050 (15)

C43	0.0533 (19)	0.0534 (18)	0.069 (2)	0.0144 (15)	0.0101 (16)	0.0003 (16)
N12	0.093 (3)	0.075 (2)	0.088 (2)	0.0220 (19)	0.018 (2)	−0.0249 (17)
N13	0.072 (2)	0.086 (2)	0.092 (2)	0.0272 (19)	0.0309 (19)	−0.0095 (18)
C12	0.047 (2)	0.065 (2)	0.078 (3)	0.0035 (17)	0.0101 (18)	−0.0026 (19)
C11	0.067 (2)	0.055 (2)	0.074 (2)	0.0001 (18)	0.0108 (19)	−0.0189 (19)

Geometric parameters (Å, °)

C21—C2	1.487 (3)	C2—N3	1.292 (3)
C21—C22	1.498 (3)	N3—N4	1.390 (3)
C21—H21A	0.9700	N4—C5	1.355 (3)
C21—H21B	0.9700	N4—C41	1.434 (3)
C22—C23	1.330 (13)	C5—O51	1.213 (3)
C22—S21	1.681 (4)	N11—C11	1.345 (3)
C23—C24	1.456 (17)	N11—C12	1.356 (3)
C23—H23	0.9300	O41—C42	1.206 (3)
C24—C25	1.345 (10)	C41—C42	1.497 (3)
C24—H24	0.9300	C41—H41A	0.9700
C25—S21	1.6807	C41—H41B	0.9700
C25—H25	0.9300	C42—C43	1.498 (3)
C23'—C24'	1.493 (13)	C43—H43A	0.9600
C23'—H23'	0.9300	C43—H43B	0.9600
C24'—C25'	1.313 (10)	C43—H43C	0.9600
C24'—H24'	0.9300	N12—C11	1.289 (3)
C25'—S21'	1.675 (11)	N12—N13	1.400 (4)
C25'—H25'	0.9300	N13—C12	1.291 (3)
N1—N11	1.376 (3)	C12—H12	0.9300
N1—C2	1.383 (3)	C11—H11	0.9300
N1—C5	1.396 (3)		
C2—C21—C22	112.6 (2)	C5—N4—N3	113.2 (2)
C2—C21—H21A	109.1	C5—N4—C41	125.5 (2)
C22—C21—H21A	109.1	N3—N4—C41	119.8 (2)
C2—C21—H21B	109.1	O51—C5—N4	130.9 (3)
C22—C21—H21B	109.1	O51—C5—N1	127.6 (3)
H21A—C21—H21B	107.8	N4—C5—N1	101.5 (2)
C23—C22—C21	123.8 (8)	C11—N11—C12	105.7 (3)
C23—C22—S21	110.7 (8)	C11—N11—N1	127.1 (3)
C21—C22—S21	125.4 (2)	C12—N11—N1	126.7 (2)
C22—C23—C24	113.9 (13)	N4—C41—C42	114.7 (2)
C22—C23—H23	123.0	N4—C41—H41A	108.6
C24—C23—H23	123.0	C42—C41—H41A	108.6
C25—C24—C23	109.4 (11)	N4—C41—H41B	108.6
C25—C24—H24	125.3	C42—C41—H41B	108.6
C23—C24—H24	125.3	H41A—C41—H41B	107.6
C24—C25—S21	112.7 (6)	O41—C42—C41	121.9 (2)
C24—C25—H25	123.6	O41—C42—C43	123.0 (3)
S21—C25—H25	123.6	C41—C42—C43	115.1 (2)
C25—S21—C22	93.23 (16)	C42—C43—H43A	109.5
C24'—C23'—H23'	125.4	C42—C43—H43B	109.5

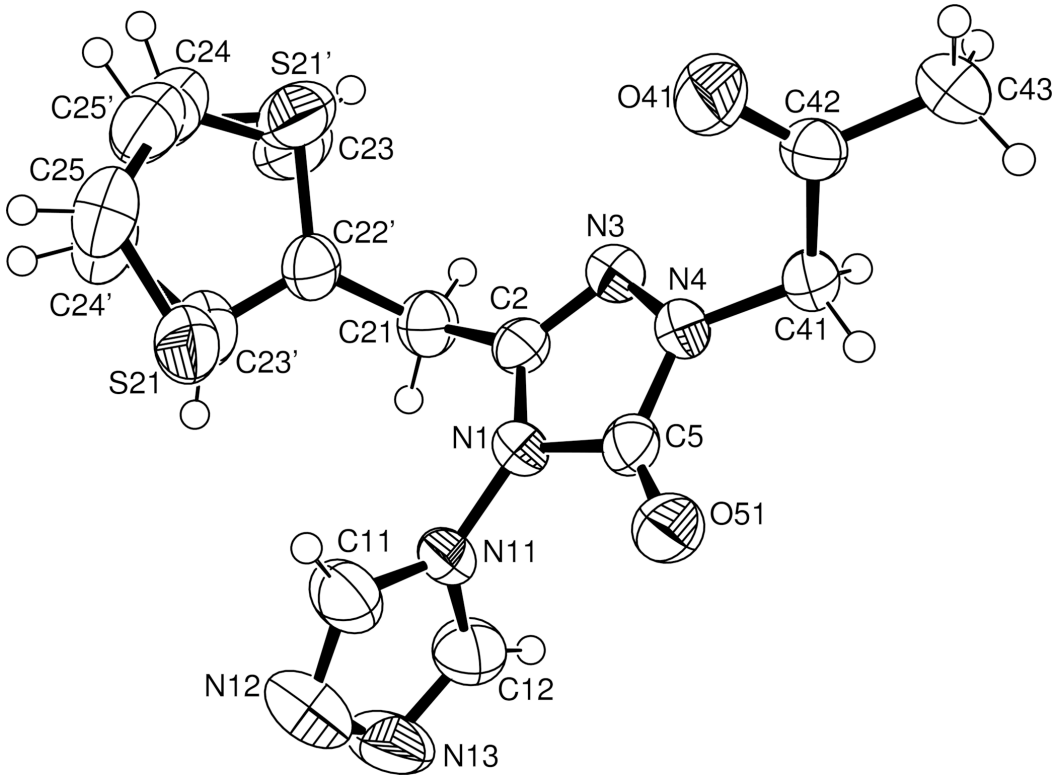
C25'—C24'—C23'	110.5 (9)	H43A—C43—H43B	109.5
C25'—C24'—H24'	124.8	C42—C43—H43C	109.5
C23'—C24'—H24'	124.8	H43A—C43—H43C	109.5
C24'—C25'—S21'	114.3 (11)	H43B—C43—H43C	109.5
C24'—C25'—H25'	122.9	C11—N12—N13	107.3 (3)
S21'—C25'—H25'	122.9	C12—N13—N12	106.6 (3)
N11—N1—C2	126.7 (2)	N13—C12—N11	110.2 (3)
N11—N1—C5	121.8 (2)	N13—C12—H12	124.9
C2—N1—C5	109.8 (2)	N11—C12—H12	124.9
N3—C2—N1	109.6 (2)	N12—C11—N11	110.2 (3)
N3—C2—C21	125.6 (3)	N12—C11—H11	124.9
N1—C2—C21	124.8 (2)	N11—C11—H11	124.9
C2—N3—N4	105.6 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C24$^{'}$—H25···N12^{i}	1.08	2.57	3.593 (9)	158
C25—H25···N12^{i}	0.93	2.57	3.409 (5)	151
C41—H41A···N3^{ii}	0.97	2.53	3.495 (3)	172
C41—H41B···O51^{iii}	0.97	2.47	3.217 (3)	134
C43—H43A···O51^{iv}	0.96	2.56	3.426 (3)	150

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

Fig. 1


C24
S21'
C25'
C23
C25
C22'
C24'
C23'
S21
C21
C2
N3
N4
C41
O41
C42
C43
N1
C5
O51
C11
N11
N12
C12
N13