IUCrData

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2-[5-(4-Fluorophenyl)-3-(4-methylphenyl)-4,5-dihydro-1*H*-pyrazol-1-yl]-4-(5-methyl-1-phenyl-1*H*-1,2,3-triazol-4-yl)thiazole

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Keywords: crystal structure; pyrazole; thiazole; 1,2,3-triazole.

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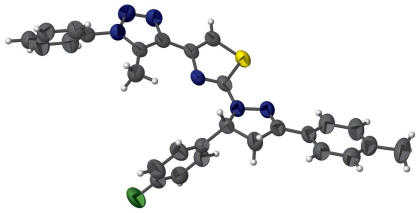
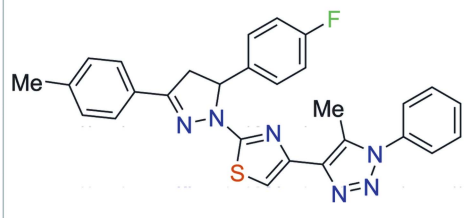
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{28}H_{23}FN_6S$, comprises phenyl (*A*), triazolyl (*B*), thiazolyl (*C*), pyrazoyl (*D*), tolyl (*E*) and fluorophenyl (*F*) rings, with twist angles between neighbouring rings pairs *A*/*B*, *B*/*C*, *C*/*D*, *D*/*E* and *D*/F of 64.6 (1), 11.7 (2), 23.5 (2), 8.2 (2) and 73.3 (1)°, respectively. A short intramolecular C—H···N contact and a weak intermolecular C—H···π interaction occur. The crystal chosen for data collection was found to be an inversion twin.

3D view



Chemical scheme



Structure description

Triazoles act as antifungal drugs and plant protection fungicides (Bonandi *et al.*, 2017). Thiazoles and pyrazoles are an essential core scaffold in many natural products and have various biological activities (Chhabria *et al.*, 2016; Faria *et al.*, 2017). As part of our studies in these areas, we now describe the synthesis and structure of the title compound.

The molecule of the title compound comprises phenyl (*A*), triazolyl (*B*), thiazolyl (*C*), pyrazoyl (*D*), tolyl (*E*) and fluorophenyl (*F*) rings (Fig. 1). The twist angles between the planes through neighbouring ring pairs *A*/*B*, *B*/*C*, *C*/*D*, *D*/*E* and *D*/*F* are 64.6 (1), 11.7 (2), 23.5 (2), 8.2 (2) and 73.3 (1)°, respectively. The packing is shown in Fig. 2. A short intramolecular C—H···N contact and a weak intermolecular C—H···π interaction occur (Table 1); the latter involves the phenyl ring bonded to the triazole ring as donor and the tolyl ring as acceptor.

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

*Cg*6 is the centroid of the C22–C27 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8*C*···N4	0.96	2.49	3.135 (5)	125
C2—H2···*Cg*6^{i}	0.93	2.93	3.451 (5)	117

Symmetry code: (i) $x-\frac{1}{2}, -y+\frac{3}{2}, -z+2$.

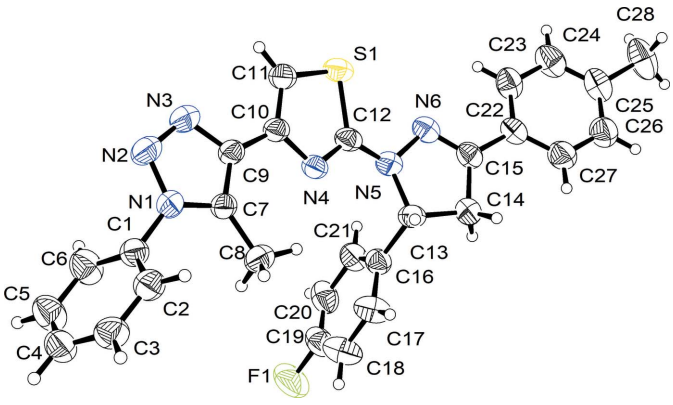


Figure 1
The molecular structure of the title compound showing 50% displacement ellipsoids.

Synthesis and crystallization

The title compound was synthesized from condensation of 5-(4-fluorophenyl)-3-*p*-tolyl-4,5-dihydro-1*H*-pyrazole-1-carbothioamide (0.63 g, 2.0 mmol) with 2-bromo-1-(5-methyl-1-phenyl-1*H*-1,2,3-triazol-4-yl)ethanone (0.56 g, 2.0 mmol) in anhydrous ethanol (20 ml) under reflux for 2 h. The crude product was recrystallized from dimethylformamide solution to give colourless crystals (74%), m.p. 241–242°C.

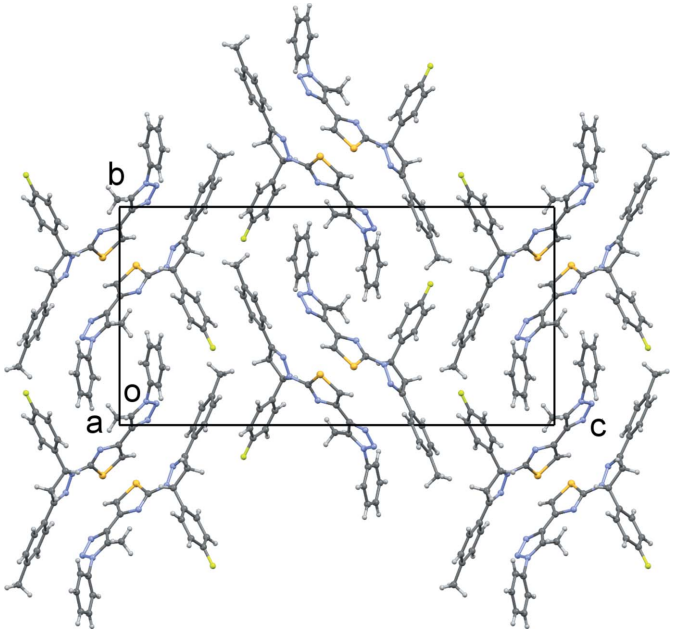


Figure 2
The crystal structure viewed down the *a*-axis direction.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{28}H_{23}FN_6S$
M_r	494.58
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	298
a, *b*, *c* (Å)	6.4930 (7), 13.8065 (10), 27.539 (2)
V (Å^3)	2468.7 (4)
Z	4
Radiation type	Mo *Kα*
μ (mm^{-1})	0.17
Crystal size (mm)	0.48 × 0.22 × 0.20
Data collection	
Diffractometer	Rigaku Oxford Diffraction SuperNova, Dual, Cu at zero, Atlas
Absorption correction	Gaussian (*CrysAlis PRO*; Rigaku OD, 2015)
T_{min}, T_{max}	0.989, 0.995
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10497, 5824, 3616
R_{int}	0.030
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.701
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.054, 0.130, 1.02
No. of reflections	5824
No. of parameters	328
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.19, −0.16
Absolute structure	Refined as an inversion twin.
Absolute structure parameter	0.39 (13)

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SHELXS* (Sheldrick, 2008), *SHELXL2018* (Sheldrick, 2015), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012), *CHEMDRAW Ultra* (Cambridge Soft, 2001).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The crystal studied was refined as a two-component inversion twin.

Funding information

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full crystallographic data

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2-[5-(4-Fluorophenyl)-3-(4-methylphenyl)-4,5-dihydro-1*H*-pyrazol-1-yl]-4-(5-methyl-1-phenyl-1*H*-1,2,3-triazol-4-yl)thiazole

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2-[5-(4-Fluorophenyl)-3-(4-methylphenyl)-4,5-dihydro-1*H*-pyrazol-1-yl]-4-(5-methyl-1-phenyl-1*H*-1,2,3-triazol-4-yl)thiazole

Crystal data

$C_{28}H_{23}FN_6S$
M_r = 494.58
Orthorhombic, $P2_12_12_1$
a = 6.4930 (7) Å
b = 13.8065 (10) Å
c = 27.539 (2) Å
V = 2468.7 (4) Å^3
Z = 4
$F(000)$ = 1032
D_x = 1.331 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2536 reflections
θ = 4.5–24.6°
μ = 0.17 mm^{-1}
T = 298 K
Block, colourless
0.48 × 0.22 × 0.20 mm

Data collection

Rigaku Oxford Diffraction SuperNova, Dual, Cu at zero, Atlas diffractometer
ω scans
Absorption correction: gaussian (CrysAlis PRO; Rigaku OD, 2015)
T_{min} = 0.989, T_{max} = 0.995
10497 measured reflections
5824 independent reflections
3616 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 29.9°, θ_{min} = 3.5°
h = −8→6
k = −18→18
l = −37→37

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.130
S = 1.02
5824 reflections
328 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0443P)^2 + 0.4094P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Absolute structure: Refined as an inversion twin.
Absolute structure parameter: 0.39 (13)

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. Refined as a twocomponent inversion twin. All hydrogen atoms were placed in calculated positions (C—H = 0.93–0.97 Å) and refined using a riding model. Their U_{iso} values were set to $1.2U_{eq}$(C) or $1.5U_{eq}$(methyl C).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	−0.4269 (7)	1.1919 (3)	1.07159 (13)	0.0559 (10)
C2	−0.6229 (7)	1.1827 (3)	1.08958 (15)	0.0649 (11)
H2	−0.678909	1.121876	1.095562	0.078*
C3	−0.7347 (7)	1.2650 (3)	1.09859 (16)	0.0717 (12)
H3	−0.867316	1.260334	1.111120	0.086*
C4	−0.6503 (9)	1.3551 (3)	1.08904 (16)	0.0739 (13)
H4	−0.725943	1.410783	1.095705	0.089*
C5	−0.4596 (9)	1.3629 (3)	1.07019 (19)	0.0849 (15)
H5	−0.404979	1.423607	1.063286	0.102*
C6	−0.3460 (8)	1.2808 (3)	1.06117 (18)	0.0797 (13)
H6	−0.214461	1.285781	1.048022	0.096*
C7	−0.3245 (6)	1.0401 (2)	1.02673 (13)	0.0511 (9)
C8	−0.5093 (7)	1.0342 (3)	0.99548 (16)	0.0691 (12)
H8A	−0.513388	1.089265	0.974237	0.104*
H8B	−0.630595	1.033504	1.015412	0.104*
H8C	−0.503877	0.975897	0.976504	0.104*
C9	−0.1463 (6)	0.9874 (2)	1.02874 (13)	0.0516 (9)
C10	−0.0736 (6)	0.9082 (3)	0.99844 (14)	0.0511 (9)
C11	0.0948 (7)	0.8538 (3)	1.00637 (14)	0.0574 (10)
H11	0.182880	0.861305	1.032728	0.069*
C12	−0.0915 (6)	0.8150 (3)	0.93398 (14)	0.0544 (10)
C13	−0.3802 (7)	0.7884 (2)	0.87594 (14)	0.0567 (10)
H13	−0.469753	0.783243	0.904477	0.068*
C14	−0.4096 (7)	0.6982 (3)	0.84381 (16)	0.0690 (12)
H14A	−0.524532	0.659290	0.855039	0.083*
H14B	−0.432842	0.716223	0.810208	0.083*
C15	−0.2083 (7)	0.6445 (3)	0.84956 (15)	0.0583 (11)
C16	−0.4171 (7)	0.8849 (3)	0.85139 (13)	0.0568 (10)
C17	−0.6006 (8)	0.9330 (3)	0.85763 (17)	0.0816 (14)
H17	−0.701415	0.905584	0.877291	0.098*
C18	−0.6390 (10)	1.0206 (4)	0.8355 (2)	0.0978 (18)
H18	−0.763844	1.052494	0.839867	0.117*
C19	−0.4880 (11)	1.0591 (3)	0.80716 (18)	0.0818 (16)
C20	−0.3074 (10)	1.0152 (3)	0.79966 (17)	0.0804 (15)
H20	−0.208150	1.043064	0.779691	0.097*
C21	−0.2713 (8)	0.9269 (3)	0.82245 (16)	0.0694 (12)
H21	−0.145671	0.895904	0.817918	0.083*

C22	−0.1595 (8)	0.5513 (3)	0.82755 (15)	0.0618 (11)
C23	0.0365 (8)	0.5127 (3)	0.83004 (18)	0.0740 (13)
H23	0.140588	0.547775	0.845171	0.089*
C24	0.0807 (9)	0.4226 (3)	0.81034 (19)	0.0843 (16)
H24	0.213884	0.398120	0.812360	0.101*
C25	−0.0720 (10)	0.3686 (3)	0.78763 (17)	0.0782 (15)
C26	−0.2671 (9)	0.4073 (3)	0.78493 (17)	0.0820 (15)
H26	−0.371342	0.372581	0.769661	0.098*
C27	−0.3102 (9)	0.4974 (3)	0.80466 (16)	0.0767 (14)
H27	−0.443203	0.521997	0.802457	0.092*
C28	−0.0244 (10)	0.2676 (4)	0.7685 (2)	0.111 (2)
H28A	−0.112090	0.253675	0.741325	0.166*
H28B	−0.048207	0.220881	0.793703	0.166*
H28C	0.116980	0.264634	0.758453	0.166*
N1	−0.3011 (5)	1.1082 (2)	1.06182 (12)	0.0562 (8)
N2	−0.1185 (6)	1.0982 (3)	1.08453 (13)	0.0734 (10)
N3	−0.0244 (6)	1.0233 (3)	1.06502 (14)	0.0708 (10)
N4	−0.1820 (5)	0.8870 (2)	0.95596 (11)	0.0517 (8)
N5	−0.1641 (5)	0.7772 (2)	0.89122 (12)	0.0595 (8)
N6	−0.0774 (6)	0.6892 (2)	0.87665 (12)	0.0603 (9)
F1	−0.5241 (6)	1.1462 (2)	0.78531 (12)	0.1226 (13)
S1	0.12603 (17)	0.76837 (7)	0.96140 (4)	0.0631 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.053 (3)	0.058 (2)	0.056 (2)	0.002 (2)	−0.0014 (19)	−0.0004 (19)
C2	0.055 (3)	0.065 (2)	0.075 (2)	−0.004 (2)	0.000 (2)	0.002 (2)
C3	0.056 (3)	0.082 (3)	0.077 (3)	0.008 (3)	0.005 (2)	−0.008 (3)
C4	0.086 (4)	0.062 (3)	0.074 (3)	0.012 (3)	−0.005 (3)	−0.008 (2)
C5	0.090 (4)	0.058 (3)	0.107 (4)	−0.001 (3)	0.010 (3)	0.006 (3)
C6	0.072 (3)	0.064 (2)	0.103 (3)	−0.006 (3)	0.017 (3)	0.006 (3)
C7	0.045 (2)	0.0479 (18)	0.060 (2)	−0.0055 (18)	−0.0047 (19)	0.0081 (17)
C8	0.056 (3)	0.075 (3)	0.077 (3)	0.006 (2)	−0.013 (2)	−0.012 (2)
C9	0.043 (2)	0.0507 (18)	0.061 (2)	−0.0044 (19)	−0.007 (2)	0.0067 (17)
C10	0.041 (2)	0.0488 (18)	0.064 (2)	−0.0031 (18)	−0.0037 (19)	0.0109 (18)
C11	0.053 (3)	0.057 (2)	0.062 (2)	0.002 (2)	−0.004 (2)	0.0069 (18)
C12	0.046 (2)	0.0502 (19)	0.067 (2)	0.0020 (19)	0.002 (2)	0.0155 (19)
C13	0.049 (2)	0.057 (2)	0.064 (2)	0.009 (2)	−0.004 (2)	0.0047 (18)
C14	0.065 (3)	0.054 (2)	0.088 (3)	0.002 (2)	−0.007 (3)	−0.002 (2)
C15	0.063 (3)	0.049 (2)	0.062 (2)	0.000 (2)	0.006 (2)	0.0085 (19)
C16	0.065 (3)	0.053 (2)	0.052 (2)	0.005 (2)	−0.003 (2)	−0.0015 (18)
C17	0.077 (4)	0.087 (3)	0.081 (3)	0.026 (3)	0.010 (3)	0.020 (3)
C18	0.105 (5)	0.093 (4)	0.096 (4)	0.039 (4)	0.001 (4)	0.016 (3)
C19	0.124 (5)	0.057 (3)	0.065 (3)	0.014 (3)	−0.019 (3)	0.003 (2)
C20	0.109 (5)	0.061 (3)	0.071 (3)	−0.006 (3)	0.002 (3)	0.004 (2)
C21	0.072 (3)	0.059 (2)	0.077 (3)	0.003 (2)	0.004 (3)	0.001 (2)
C22	0.070 (3)	0.050 (2)	0.065 (2)	0.005 (2)	0.006 (2)	0.0065 (19)

C23	0.074 (4)	0.061 (3)	0.088 (3)	−0.003 (2)	0.016 (3)	−0.006 (2)
C24	0.079 (4)	0.068 (3)	0.106 (4)	0.010 (3)	0.032 (3)	0.002 (3)
C25	0.099 (4)	0.059 (3)	0.077 (3)	−0.001 (3)	0.023 (3)	0.000 (2)
C26	0.097 (4)	0.068 (3)	0.081 (3)	0.000 (3)	−0.009 (3)	−0.005 (3)
C27	0.087 (4)	0.066 (3)	0.077 (3)	0.009 (3)	−0.008 (3)	−0.006 (2)
C28	0.150 (6)	0.062 (3)	0.120 (4)	−0.002 (3)	0.042 (4)	−0.017 (3)
N1	0.048 (2)	0.0557 (17)	0.0654 (18)	−0.0025 (16)	−0.0046 (17)	−0.0033 (17)
N2	0.056 (2)	0.083 (2)	0.081 (2)	0.006 (2)	−0.019 (2)	−0.016 (2)
N3	0.056 (2)	0.074 (2)	0.082 (2)	0.0069 (19)	−0.019 (2)	−0.009 (2)
N4	0.0483 (19)	0.0456 (15)	0.0613 (18)	0.0026 (15)	−0.0022 (16)	0.0077 (15)
N5	0.056 (2)	0.0556 (17)	0.0673 (19)	0.0098 (17)	−0.0044 (17)	−0.0025 (16)
N6	0.062 (2)	0.0547 (17)	0.0644 (19)	0.0076 (18)	0.0068 (18)	0.0029 (17)
F1	0.179 (4)	0.0690 (17)	0.120 (2)	0.023 (2)	−0.030 (2)	0.0235 (17)
S1	0.0522 (6)	0.0618 (5)	0.0754 (6)	0.0127 (5)	−0.0014 (6)	0.0094 (5)

Geometric parameters (Å, º)

C1—C6	1.366 (5)	C14—H14A	0.9700
C1—C2	1.372 (6)	C14—H14B	0.9700
C1—N1	1.440 (5)	C15—N6	1.288 (5)
C2—C3	1.371 (6)	C15—C22	1.458 (5)
C2—H2	0.9300	C16—C21	1.367 (6)
C3—C4	1.385 (6)	C16—C17	1.374 (6)
C3—H3	0.9300	C17—C18	1.378 (6)
C4—C5	1.347 (7)	C17—H17	0.9300
C4—H4	0.9300	C18—C19	1.361 (8)
C5—C6	1.375 (6)	C18—H18	0.9300
C5—H5	0.9300	C19—C20	1.336 (8)
C6—H6	0.9300	C19—F1	1.366 (5)
C7—N1	1.357 (4)	C20—C21	1.391 (6)
C7—C9	1.368 (5)	C20—H20	0.9300
C7—C8	1.479 (6)	C21—H21	0.9300
C8—H8A	0.9600	C22—C23	1.381 (6)
C8—H8B	0.9600	C22—C27	1.381 (6)
C8—H8C	0.9600	C23—C24	1.387 (6)
C9—N3	1.368 (5)	C23—H23	0.9300
C9—C10	1.454 (5)	C24—C25	1.389 (7)
C10—C11	1.344 (5)	C24—H24	0.9300
C10—N4	1.396 (5)	C25—C26	1.377 (7)
C11—S1	1.722 (4)	C25—C28	1.522 (6)
C11—H11	0.9300	C26—C27	1.385 (6)
C12—N4	1.304 (5)	C26—H26	0.9300
C12—N5	1.371 (5)	C27—H27	0.9300
C12—S1	1.726 (4)	C28—H28A	0.9600
C13—N5	1.473 (5)	C28—H28B	0.9600
C13—C16	1.513 (5)	C28—H28C	0.9600
C13—C14	1.540 (5)	N1—N2	1.348 (5)
C13—H13	0.9800	N2—N3	1.315 (5)

C14—C15	1.511 (6)	N5—N6	1.398 (4)
C6—C1—C2	121.1 (4)	C21—C16—C17	117.9 (4)
C6—C1—N1	117.6 (4)	C21—C16—C13	121.7 (4)
C2—C1—N1	121.3 (4)	C17—C16—C13	120.4 (4)
C3—C2—C1	118.7 (4)	C16—C17—C18	121.7 (5)
C3—C2—H2	120.7	C16—C17—H17	119.1
C1—C2—H2	120.7	C18—C17—H17	119.1
C2—C3—C4	120.1 (4)	C19—C18—C17	117.8 (5)
C2—C3—H3	120.0	C19—C18—H18	121.1
C4—C3—H3	120.0	C17—C18—H18	121.1
C5—C4—C3	120.5 (4)	C20—C19—C18	123.0 (5)
C5—C4—H4	119.7	C20—C19—F1	118.8 (6)
C3—C4—H4	119.7	C18—C19—F1	118.2 (6)
C4—C5—C6	119.8 (5)	C19—C20—C21	118.3 (5)
C4—C5—H5	120.1	C19—C20—H20	120.8
C6—C5—H5	120.1	C21—C20—H20	120.8
C1—C6—C5	119.8 (5)	C16—C21—C20	121.3 (5)
C1—C6—H6	120.1	C16—C21—H21	119.4
C5—C6—H6	120.1	C20—C21—H21	119.4
N1—C7—C9	104.2 (3)	C23—C22—C27	117.9 (4)
N1—C7—C8	122.9 (4)	C23—C22—C15	121.3 (4)
C9—C7—C8	132.9 (4)	C27—C22—C15	120.8 (4)
C7—C8—H8A	109.5	C22—C23—C24	121.1 (5)
C7—C8—H8B	109.5	C22—C23—H23	119.4
H8A—C8—H8B	109.5	C24—C23—H23	119.4
C7—C8—H8C	109.5	C23—C24—C25	120.6 (5)
H8A—C8—H8C	109.5	C23—C24—H24	119.7
H8B—C8—H8C	109.5	C25—C24—H24	119.7
N3—C9—C7	109.1 (3)	C26—C25—C24	118.2 (4)
N3—C9—C10	120.2 (4)	C26—C25—C28	121.6 (5)
C7—C9—C10	130.6 (4)	C24—C25—C28	120.2 (6)
C11—C10—N4	115.4 (3)	C25—C26—C27	120.9 (5)
C11—C10—C9	126.2 (4)	C25—C26—H26	119.6
N4—C10—C9	118.4 (3)	C27—C26—H26	119.6
C10—C11—S1	111.2 (3)	C22—C27—C26	121.3 (5)
C10—C11—H11	124.4	C22—C27—H27	119.4
S1—C11—H11	124.4	C26—C27—H27	119.4
N4—C12—N5	122.3 (4)	C25—C28—H28A	109.5
N4—C12—S1	116.7 (3)	C25—C28—H28B	109.5
N5—C12—S1	121.0 (3)	H28A—C28—H28B	109.5
N5—C13—C16	111.8 (3)	C25—C28—H28C	109.5
N5—C13—C14	101.4 (3)	H28A—C28—H28C	109.5
C16—C13—C14	115.8 (3)	H28B—C28—H28C	109.5
N5—C13—H13	109.2	N2—N1—C7	110.9 (3)
C16—C13—H13	109.2	N2—N1—C1	119.7 (3)
C14—C13—H13	109.2	C7—N1—C1	128.7 (3)
C15—C14—C13	103.3 (4)	N3—N2—N1	107.5 (3)

C15—C14—H14A	111.1	N2—N3—C9	108.3 (3)
C13—C14—H14A	111.1	C12—N4—C10	108.8 (3)
C15—C14—H14B	111.1	C12—N5—N6	116.0 (3)
C13—C14—H14B	111.1	C12—N5—C13	122.2 (3)
H14A—C14—H14B	109.1	N6—N5—C13	113.1 (3)
N6—C15—C22	121.4 (4)	C15—N6—N5	108.5 (3)
N6—C15—C14	113.4 (3)	C11—S1—C12	87.9 (2)
C22—C15—C14	125.3 (4)		

Hydrogen-bond geometry (Å, º)

Cg6 is the centroid of the C22–C27 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8*C*···N4	0.96	2.49	3.135 (5)	125
C2—H2···*Cg*6^{i}	0.93	2.93	3.451 (5)	117

Symmetry code: (i) $x-1/2, -y+3/2, -z+2$.