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Ethyl 3-({[(4-methylphenyl)carbamoyl]methyl}-sulfanyl)-5,6-diphenylpyridazine-4-carboxylate

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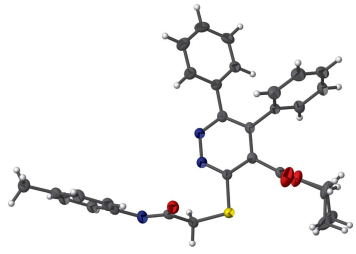
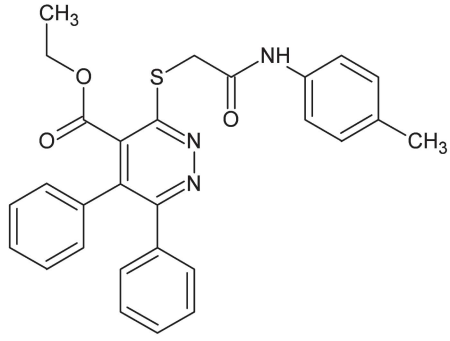
Structural data: full structural data are available from iucrdata.iucr.org

The packing in the crystal of the title molecule, $C_{28}H_{25}N_3O_3S$, is aided by intermolecular N—H···O and C—H···O hydrogen bonds. In the crystal, the ethyl group of the ester is disordered over two sets of sites with refined occupancies of 0.760 (8) and 0.240 (8).

3D view



Chemical scheme



Structure description

The broad spectrum of biological activities associated with many pyridazine derivatives are well known. Some of them are reported to exhibit antiviral, anticancer, anti-tuberculosis and antimicrobial activity (Butnariu & Mangalagiu, 2009). Others reported to possess promising pharmacological activity for use as anti-hypertensive, cardiotonic and antinociceptive agents as well as coagulants (Alonazy *et al.*, 2009). As part of our studies in this area, we undertook the synthesis of the title compound (Fig. 1) and determine its crystal structure.

The phenyl rings C17–C22 and C23–C28 make dihedral angles of 77.09 (11) and 45.86 (12)°, respectively, with the pyridazine ring. All geometric parameters are within normal ranges.

In the crystal, molecules are linked by N—H···O and C—H···O hydrogen bonds (Table 1, Fig. 2 and Fig. 3). No π–π stacking interactions are observed but C—H···π interactions help to consolidate the packing (Table 1).

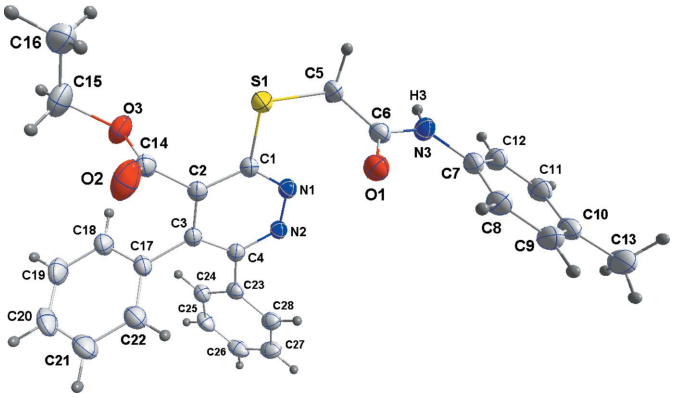


Figure 1
The title molecule with the labeling scheme and 50% probability ellipsoids.

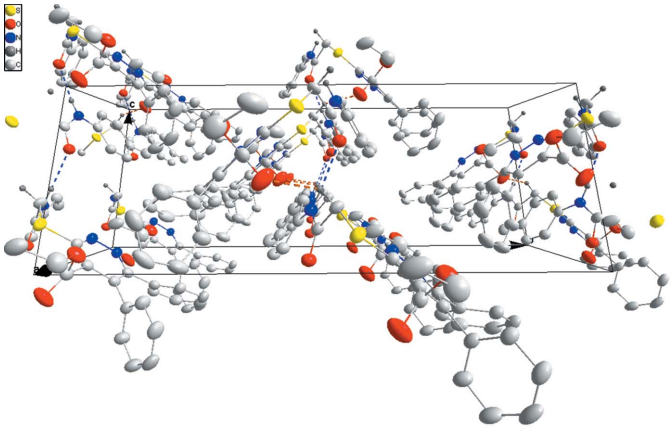


Figure 2
Packing viewed down the *a* axis with N—H···O and C—H···O hydrogen bonds shown, respectively, as blue and orange dotted lines.

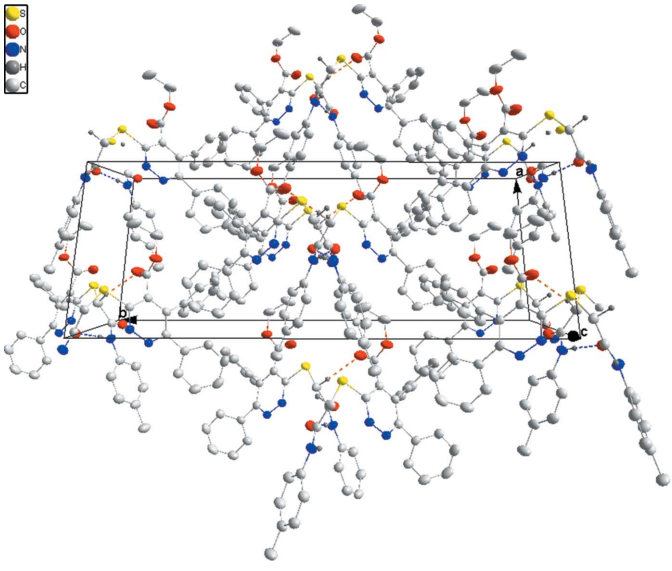


Figure 3
Packing viewed down the *c* axis with N—H···O and C—H···O hydrogen bonds shown, respectively, as blue and orange dotted lines.

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

*Cg*1, *Cg*2 and *Cg*4 are the centroids of the pyridazine (N1/N2/C1–C4), 4-methylphenyl (C7–C12) and phenyl (C23–C28) rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3···O1^{i}	0.87	2.21	3.073 (3)	174
C5—H5*B*···O2^{i}	0.99	2.36	3.220 (4)	144
C11—H11···O2^{ii}	0.95	2.43	3.263 (4)	146
C20—H20···*Cg*4^{iii}	0.95	2.61	3.495 (3)	155
C26—H26···*Cg*1^{iv}	0.95	2.80	3.556 (3)	137
C28—H28···*Cg*2^{v}	0.95	2.66	3.484 (3)	146

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

Synthesis and crystallization

A mixture of ethyl 2,3-dihydro-5,6-diphenyl-3-thioxopyridazine-4-carboxylate (1.68 g, 5 mmol), sodium acetate trihydrate (0.68 g, 5 mmol) and chloro-*N*-(4-methylphenyl)acetamide (0.92 g, 5 mmol) in ethanol (30 ml) was heated under reflux for 2 h. The product which separated on cooling was collected and recrystallized from ethanol to give colorless crystals of the title compound. Yield: 2.10 g (87%), m.p. 433–434 K. IR (KBr) ν = 3300 (NH), 1720 (C═O, ester), 1670 (C═O, carbamoyl), ^{1}H NMR ($CDCl_3$): δ 9.0 (*s*, 1H, NH), 6.9–7.6 (*m*, 14H, Ar—H), 4.1–4.4 (*q*, 2H, OCH_2), 4.0 (*s*, 2H,

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{28}H_{25}N_3O_3S$
M_r	483.57
Crystal system, space group	Monoclinic, *Cc*
Temperature (K)	150
a, *b*, *c* (Å)	10.2254 (3), 26.6695 (9), 9.9210 (3)
β (°)	110.718 (1)
V (Å^3)	2530.56 (14)
Z	4
Radiation type	Cu *K*α
μ (mm^{-1})	1.41
Crystal size (mm)	0.19 × 0.19 × 0.10
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.81, 0.88
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13580, 3992, 3898
R_{int}	0.029
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.593
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.028, 0.071, 1.04
No. of reflections	3992
No. of parameters	326
No. of restraints	6
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.30, −0.15
Absolute structure	Flack (1983), 1791 Friedel pairs
Absolute structure parameter	0.032 (17)

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

SCH_2), 2.2 (*s*, 3H, CH_3), 1.0–1.3 (*t*, 3H, CH_3 of ester). Elemental analysis calculated for $C_{28}H_{25}N_3O_3S$ (%): C, 69.54; H, 5.21; N, 8.69; S, 6.63. Found (%): C, 69.19; H, 5.14; N, 8.61; S, 6.70.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The ethoxy group of the ester is disordered over two sets of sites with an occupancy ratio of 0.760 (8):0.240 (8) and these were modeled with restraints that their geometries be comparable. In the disorder model, atoms O3 and O3*A* were kept in the same position using EXYZ and EADP commands.

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x160479 [doi:10.1107/S241431461600479X]

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Crystal data

$C_{28}H_{25}N_3O_3S$
M_r = 483.57
Monoclinic, *Cc*
a = 10.2254 (3) Å
b = 26.6695 (9) Å
c = 9.9210 (3) Å
β = 110.718 (1)°
V = 2530.56 (14) Å^3
Z = 4
F(000) = 1016
D_x = 1.269 Mg m^{-3}
Cu *K*α radiation, λ = 1.54178 Å
Cell parameters from 9986 reflections
θ = 3.3–66.2°
μ = 1.41 mm^{-1}
T = 150 K
Plate, colourless
0.19 × 0.19 × 0.10 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC IμS micro–focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
T_{min} = 0.81, T_{max} = 0.88
13580 measured reflections
3992 independent reflections
3898 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 66.2°, θ_{min} = 3.3°
h = −12→10
k = −31→31
l = −11→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.071
S = 1.04
3992 reflections
326 parameters
6 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0428P)^2 + 0.5908P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}
Extinction correction: *SHELXL2014* (Sheldrick, 2015b), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00168 (17)
Absolute structure: Flack (1983), 1791 Friedel pairs
Absolute structure parameter: 0.032 (17)

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
S1	0.74550 (6)	0.46021 (2)	0.76373 (6)	0.03062 (16)	
O1	0.48527 (18)	0.52387 (7)	0.63741 (18)	0.0330 (4)	
O2	0.8388 (2)	0.41894 (9)	0.4697 (3)	0.0524 (6)	
N1	0.5118 (2)	0.40599 (7)	0.6734 (2)	0.0279 (4)	
N2	0.4255 (2)	0.37053 (7)	0.5934 (2)	0.0267 (4)	
N3	0.4189 (2)	0.52041 (8)	0.8345 (2)	0.0306 (5)	
H3	0.4400	0.5057	0.9177	0.037*	
C1	0.6375 (2)	0.41215 (8)	0.6639 (2)	0.0242 (5)	
C2	0.6853 (3)	0.38241 (9)	0.5729 (2)	0.0249 (5)	
C3	0.5952 (2)	0.34723 (9)	0.4866 (2)	0.0246 (5)	
C4	0.4638 (2)	0.34225 (9)	0.5020 (2)	0.0255 (5)	
C5	0.6394 (3)	0.48489 (9)	0.8579 (3)	0.0291 (5)	
H5A	0.6128	0.4571	0.9090	0.035*	
H5B	0.6960	0.5089	0.9315	0.035*	
C6	0.5068 (3)	0.51128 (8)	0.7625 (3)	0.0272 (5)	
C7	0.2813 (2)	0.54069 (9)	0.7795 (3)	0.0292 (6)	
C8	0.2266 (3)	0.56605 (9)	0.6500 (3)	0.0336 (6)	
H8	0.2820	0.5716	0.5921	0.040*	
C9	0.0888 (3)	0.58348 (10)	0.6052 (3)	0.0358 (6)	
H9	0.0513	0.6006	0.5157	0.043*	
C10	0.0053 (3)	0.57657 (10)	0.6875 (3)	0.0339 (6)	
C11	0.0634 (3)	0.55100 (10)	0.8176 (3)	0.0365 (6)	
H11	0.0080	0.5454	0.8755	0.044*	
C12	0.1995 (3)	0.53361 (9)	0.8645 (3)	0.0326 (6)	
H12	0.2373	0.5168	0.9546	0.039*	
C13	−0.1412 (3)	0.59740 (11)	0.6421 (3)	0.0434 (7)	
H13A	−0.2041	0.5718	0.6556	0.065*	
H13B	−0.1725	0.6071	0.5403	0.065*	
H13C	−0.1419	0.6268	0.7009	0.065*	
C14	0.8249 (3)	0.39184 (9)	0.5604 (3)	0.0273 (5)	
O3_a	0.92581 (19)	0.36604 (8)	0.6547 (2)	0.0412 (5)	0.760 (8)
C15_a	1.0650 (10)	0.3697 (8)	0.6450 (15)	0.0487 (9)	0.760 (8)
H15A_a	1.0557	0.3696	0.5422	0.058*	0.760 (8)
H15B_a	1.1205	0.3399	0.6914	0.058*	0.760 (8)
C16_a	1.1403 (5)	0.4156 (2)	0.7147 (5)	0.0548 (14)	0.760 (8)
H16A_a	1.2322	0.4165	0.7047	0.082*	0.760 (8)
H16B_a	1.1522	0.4154	0.8172	0.082*	0.760 (8)
H16C_a	1.0863	0.4452	0.6684	0.082*	0.760 (8)
O3A_b	0.92581 (19)	0.36604 (8)	0.6547 (2)	0.0412 (5)	0.240 (8)

C15A_b	1.064 (3)	0.368 (3)	0.635 (4)	0.0487 (9)	0.240 (8)
H15C_b	1.0904	0.3341	0.6120	0.058*	0.240 (8)
H15D_b	1.0594	0.3908	0.5548	0.058*	0.240 (8)
C16A_b	1.1697 (16)	0.3864 (8)	0.7724 (17)	0.0548 (14)	0.240 (8)
H16D_b	1.2616	0.3881	0.7625	0.082*	0.240 (8)
H16E_b	1.1741	0.3634	0.8508	0.082*	0.240 (8)
H16F_b	1.1428	0.4199	0.7941	0.082*	0.240 (8)
C17	0.6349 (3)	0.31765 (9)	0.3795 (3)	0.0285 (5)	
C18	0.7382 (3)	0.28145 (10)	0.4234 (3)	0.0365 (6)	
H18	0.7855	0.2752	0.5232	0.044*	
C19	0.7725 (3)	0.25428 (12)	0.3210 (4)	0.0445 (7)	
H19	0.8421	0.2289	0.3508	0.053*	
C20	0.7055 (3)	0.26401 (12)	0.1760 (3)	0.0466 (8)	
H20	0.7293	0.2454	0.1063	0.056*	
C21	0.6050 (3)	0.30046 (13)	0.1328 (3)	0.0459 (7)	
H21	0.5603	0.3075	0.0330	0.055*	
C22	0.5680 (3)	0.32730 (11)	0.2339 (3)	0.0391 (6)	
H22	0.4970	0.3522	0.2034	0.047*	
C23	0.3571 (3)	0.30472 (9)	0.4227 (2)	0.0267 (5)	
C24	0.3919 (3)	0.25438 (10)	0.4137 (3)	0.0315 (5)	
H24	0.4869	0.2440	0.4522	0.038*	
C25	0.2879 (3)	0.21976 (10)	0.3485 (3)	0.0380 (6)	
H25	0.3116	0.1855	0.3436	0.046*	
C26	0.1498 (3)	0.23462 (11)	0.2908 (3)	0.0414 (7)	
H26	0.0789	0.2106	0.2468	0.050*	
C27	0.1147 (3)	0.28431 (11)	0.2969 (3)	0.0392 (6)	
H27	0.0199	0.2946	0.2555	0.047*	
C28	0.2182 (3)	0.31937 (10)	0.3637 (3)	0.0319 (5)	
H28	0.1937	0.3535	0.3689	0.038*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0250 (3)	0.0342 (3)	0.0338 (3)	−0.0036 (3)	0.0117 (2)	−0.0090 (2)
O1	0.0343 (10)	0.0380 (9)	0.0290 (9)	0.0020 (8)	0.0142 (7)	0.0001 (7)
O2	0.0378 (12)	0.0637 (13)	0.0644 (14)	0.0072 (10)	0.0289 (10)	0.0290 (11)
N1	0.0260 (11)	0.0286 (10)	0.0308 (10)	−0.0014 (8)	0.0123 (8)	−0.0026 (8)
N2	0.0257 (11)	0.0271 (10)	0.0286 (10)	−0.0012 (8)	0.0113 (8)	−0.0025 (8)
N3	0.0303 (12)	0.0351 (11)	0.0273 (10)	0.0063 (9)	0.0115 (9)	0.0015 (8)
C1	0.0235 (12)	0.0254 (12)	0.0242 (11)	0.0005 (9)	0.0090 (9)	−0.0008 (9)
C2	0.0266 (12)	0.0254 (11)	0.0237 (11)	0.0024 (9)	0.0099 (9)	0.0031 (9)
C3	0.0257 (12)	0.0254 (11)	0.0240 (11)	0.0035 (9)	0.0105 (9)	0.0023 (9)
C4	0.0272 (13)	0.0261 (11)	0.0246 (11)	0.0028 (9)	0.0109 (9)	0.0043 (9)
C5	0.0287 (13)	0.0333 (13)	0.0265 (12)	0.0007 (10)	0.0111 (10)	−0.0088 (10)
C6	0.0285 (13)	0.0261 (12)	0.0271 (13)	−0.0027 (10)	0.0098 (9)	−0.0063 (10)
C7	0.0291 (15)	0.0275 (11)	0.0314 (13)	0.0015 (10)	0.0113 (11)	−0.0063 (9)
C8	0.0349 (15)	0.0375 (13)	0.0295 (13)	0.0028 (11)	0.0127 (10)	−0.0018 (10)
C9	0.0350 (15)	0.0402 (15)	0.0290 (13)	0.0062 (11)	0.0076 (11)	−0.0020 (10)

C10	0.0293 (14)	0.0333 (13)	0.0376 (14)	0.0013 (11)	0.0100 (10)	−0.0107 (11)
C11	0.0352 (15)	0.0376 (14)	0.0408 (14)	−0.0017 (12)	0.0186 (12)	−0.0071 (11)
C12	0.0341 (15)	0.0341 (13)	0.0317 (13)	0.0025 (11)	0.0142 (11)	−0.0005 (10)
C13	0.0308 (15)	0.0493 (16)	0.0464 (16)	0.0056 (12)	0.0091 (12)	−0.0076 (13)
C14	0.0275 (13)	0.0271 (12)	0.0293 (12)	0.0015 (10)	0.0124 (10)	−0.0020 (10)
O3_a	0.0258 (10)	0.0542 (12)	0.0453 (11)	0.0064 (8)	0.0147 (8)	0.0137 (9)
C15_a	0.0270 (15)	0.061 (2)	0.062 (3)	0.0052 (14)	0.0203 (15)	0.0056 (18)
C16_a	0.037 (2)	0.088 (4)	0.043 (3)	−0.019 (2)	0.0196 (19)	−0.015 (2)
O3A_b	0.0258 (10)	0.0542 (12)	0.0453 (11)	0.0064 (8)	0.0147 (8)	0.0137 (9)
C15A_b	0.0270 (15)	0.061 (2)	0.062 (3)	0.0052 (14)	0.0203 (15)	0.0056 (18)
C16A_b	0.037 (2)	0.088 (4)	0.043 (3)	−0.019 (2)	0.0196 (19)	−0.015 (2)
C17	0.0275 (12)	0.0308 (12)	0.0312 (12)	−0.0044 (10)	0.0155 (10)	−0.0072 (10)
C18	0.0347 (15)	0.0396 (14)	0.0382 (14)	0.0010 (12)	0.0168 (11)	−0.0071 (11)
C19	0.0386 (16)	0.0438 (16)	0.0581 (18)	0.0013 (13)	0.0258 (14)	−0.0138 (13)
C20	0.0488 (18)	0.0528 (17)	0.0504 (18)	−0.0160 (15)	0.0326 (15)	−0.0261 (14)
C21	0.0483 (18)	0.0602 (19)	0.0327 (14)	−0.0096 (15)	0.0188 (12)	−0.0128 (13)
C22	0.0397 (16)	0.0488 (16)	0.0315 (14)	−0.0035 (12)	0.0161 (11)	−0.0059 (12)
C23	0.0282 (13)	0.0312 (12)	0.0237 (11)	−0.0037 (10)	0.0127 (9)	−0.0001 (9)
C24	0.0345 (14)	0.0318 (13)	0.0315 (13)	−0.0021 (11)	0.0158 (11)	−0.0042 (10)
C25	0.0489 (17)	0.0328 (14)	0.0374 (14)	−0.0093 (12)	0.0217 (13)	−0.0110 (11)
C26	0.0442 (17)	0.0499 (17)	0.0316 (13)	−0.0202 (14)	0.0151 (11)	−0.0118 (12)
C27	0.0307 (14)	0.0535 (17)	0.0315 (13)	−0.0067 (12)	0.0087 (11)	−0.0001 (12)
C28	0.0311 (14)	0.0373 (13)	0.0279 (12)	−0.0020 (11)	0.0112 (10)	0.0024 (10)

Geometric parameters (Å, º)

S1—C1	1.752 (2)	C15_a—C16_a	1.481 (15)
S1—C5	1.789 (2)	C15_a—H15A_a	0.9900
O1—C6	1.228 (3)	C15_a—H15B_a	0.9900
O2—C14	1.201 (3)	C16_a—H16A_a	0.9800
N1—C1	1.332 (3)	C16_a—H16B_a	0.9800
N1—N2	1.344 (3)	C16_a—H16C_a	0.9800
N2—C4	1.341 (3)	C15A_b—C16A_b	1.49 (3)
N3—C6	1.354 (3)	C15A_b—H15C_b	0.9900
N3—C7	1.423 (3)	C15A_b—H15D_b	0.9900
N3—H3	0.8702	C16A_b—H16D_b	0.9800
C1—C2	1.412 (3)	C16A_b—H16E_b	0.9800
C2—C3	1.380 (3)	C16A_b—H16F_b	0.9800
C2—C14	1.497 (3)	C17—C18	1.382 (4)
C3—C4	1.411 (3)	C17—C22	1.386 (4)
C3—C17	1.491 (3)	C18—C19	1.390 (4)
C4—C23	1.484 (3)	C18—H18	0.9500
C5—C6	1.523 (3)	C19—C20	1.382 (5)
C5—H5A	0.9900	C19—H19	0.9500
C5—H5B	0.9900	C20—C21	1.369 (5)
C7—C8	1.383 (4)	C20—H20	0.9500
C7—C12	1.395 (4)	C21—C22	1.390 (4)
C8—C9	1.398 (4)	C21—H21	0.9500

C8—H8	0.9500	C22—H22	0.9500
C9—C10	1.387 (4)	C23—C28	1.387 (4)
C9—H9	0.9500	C23—C24	1.400 (4)
C10—C11	1.394 (4)	C24—C25	1.384 (4)
C10—C13	1.509 (4)	C24—H24	0.9500
C11—C12	1.382 (4)	C25—C26	1.381 (4)
C11—H11	0.9500	C25—H25	0.9500
C12—H12	0.9500	C26—C27	1.380 (5)
C13—H13A	0.9800	C26—H26	0.9500
C13—H13B	0.9800	C27—C28	1.392 (4)
C13—H13C	0.9800	C27—H27	0.9500
C14—O3_a	1.316 (3)	C28—H28	0.9500
O3_a—C15_a	1.463 (9)		

C1—S1—C5	100.79 (11)	O3_a—C15_a—H15A_a	109.1
C1—N1—N2	119.57 (19)	C16_a—C15_a—H15A_a	109.1
C4—N2—N1	120.5 (2)	O3_a—C15_a—H15B_a	109.1
C6—N3—C7	128.1 (2)	C16_a—C15_a—H15B_a	109.1
C6—N3—H3	115.5	H15A_a—C15_a—H15B_a	107.9
C7—N3—H3	114.5	C15_a—C16_a—H16A_a	109.5
N1—C1—C2	122.5 (2)	C15_a—C16_a—H16B_a	109.5
N1—C1—S1	118.76 (17)	H16A_a—C16_a—H16B_a	109.5
C2—C1—S1	118.76 (18)	C15_a—C16_a—H16C_a	109.5
C3—C2—C1	118.2 (2)	H16A_a—C16_a—H16C_a	109.5
C3—C2—C14	120.6 (2)	H16B_a—C16_a—H16C_a	109.5
C1—C2—C14	120.9 (2)	C16A_b—C15A_b—H15C_b	110.2
C2—C3—C4	116.7 (2)	C16A_b—C15A_b—H15D_b	110.2
C2—C3—C17	120.8 (2)	H15C_b—C15A_b—H15D_b	108.5
C4—C3—C17	122.5 (2)	C15A_b—C16A_b—H16D_b	109.5
N2—C4—C3	122.5 (2)	C15A_b—C16A_b—H16E_b	109.5
N2—C4—C23	113.7 (2)	H16D_b—C16A_b—H16E_b	109.5
C3—C4—C23	123.8 (2)	C15A_b—C16A_b—H16F_b	109.5
C6—C5—S1	114.61 (17)	H16D_b—C16A_b—H16F_b	109.5
C6—C5—H5A	108.6	H16E_b—C16A_b—H16F_b	109.5
S1—C5—H5A	108.6	C18—C17—C22	119.9 (2)
C6—C5—H5B	108.6	C18—C17—C3	121.0 (2)
S1—C5—H5B	108.6	C22—C17—C3	119.1 (2)
H5A—C5—H5B	107.6	C17—C18—C19	119.7 (3)
O1—C6—N3	124.7 (2)	C17—C18—H18	120.2
O1—C6—C5	123.8 (2)	C19—C18—H18	120.2
N3—C6—C5	111.5 (2)	C20—C19—C18	120.2 (3)
C8—C7—C12	119.7 (2)	C20—C19—H19	119.9
C8—C7—N3	124.2 (2)	C18—C19—H19	119.9
C12—C7—N3	116.1 (2)	C21—C20—C19	120.0 (3)
C7—C8—C9	119.2 (2)	C21—C20—H20	120.0
C7—C8—H8	120.4	C19—C20—H20	120.0
C9—C8—H8	120.4	C20—C21—C22	120.4 (3)
C10—C9—C8	122.0 (2)	C20—C21—H21	119.8

C10—C9—H9	119.0	C22—C21—H21	119.8
C8—C9—H9	119.0	C17—C22—C21	119.7 (3)
C9—C10—C11	117.5 (2)	C17—C22—H22	120.1
C9—C10—C13	121.9 (3)	C21—C22—H22	120.1
C11—C10—C13	120.6 (3)	C28—C23—C24	119.3 (2)
C12—C11—C10	121.6 (3)	C28—C23—C4	119.0 (2)
C12—C11—H11	119.2	C24—C23—C4	121.7 (2)
C10—C11—H11	119.2	C25—C24—C23	119.9 (2)
C11—C12—C7	119.9 (2)	C25—C24—H24	120.0
C11—C12—H12	120.0	C23—C24—H24	120.0
C7—C12—H12	120.0	C26—C25—C24	120.4 (3)
C10—C13—H13A	109.5	C26—C25—H25	119.8
C10—C13—H13B	109.5	C24—C25—H25	119.8
H13A—C13—H13B	109.5	C27—C26—C25	120.1 (3)
C10—C13—H13C	109.5	C27—C26—H26	120.0
H13A—C13—H13C	109.5	C25—C26—H26	120.0
H13B—C13—H13C	109.5	C26—C27—C28	120.0 (3)
O2—C14—O3_a	125.2 (2)	C26—C27—H27	120.0
O2—C14—C2	122.2 (2)	C28—C27—H27	120.0
O3_a—C14—C2	112.6 (2)	C23—C28—C27	120.3 (3)
C14—O3_a—C15_a	117.0 (9)	C23—C28—H28	119.9
O3_a—C15_a—C16_a	112.4 (10)	C27—C28—H28	119.9

C1—N1—N2—C4	−1.6 (3)	C8—C7—C12—C11	1.4 (4)
N2—N1—C1—C2	−0.5 (3)	N3—C7—C12—C11	−178.4 (2)
N2—N1—C1—S1	177.52 (16)	C3—C2—C14—O2	82.4 (3)
C5—S1—C1—N1	2.3 (2)	C1—C2—C14—O2	−92.1 (3)
C5—S1—C1—C2	−179.63 (18)	C3—C2—C14—O3_a	−95.3 (3)
N1—C1—C2—C3	2.8 (3)	C1—C2—C14—O3_a	90.2 (3)
S1—C1—C2—C3	−175.15 (17)	O2—C14—O3_a—C15_a	−2.0 (7)
N1—C1—C2—C14	177.4 (2)	C2—C14—O3_a—C15_a	175.7 (6)
S1—C1—C2—C14	−0.6 (3)	C14—O3_a—C15_a—C16_a	81.2 (11)
C1—C2—C3—C4	−3.0 (3)	C2—C3—C17—C18	70.0 (3)
C14—C2—C3—C4	−177.6 (2)	C4—C3—C17—C18	−112.2 (3)
C1—C2—C3—C17	174.9 (2)	C2—C3—C17—C22	−109.2 (3)
C14—C2—C3—C17	0.3 (3)	C4—C3—C17—C22	68.6 (3)
N1—N2—C4—C3	1.3 (3)	C22—C17—C18—C19	−1.2 (4)
N1—N2—C4—C23	179.63 (19)	C3—C17—C18—C19	179.7 (3)
C2—C3—C4—N2	1.1 (3)	C17—C18—C19—C20	1.2 (4)
C17—C3—C4—N2	−176.7 (2)	C18—C19—C20—C21	−0.1 (5)
C2—C3—C4—C23	−177.1 (2)	C19—C20—C21—C22	−1.1 (5)
C17—C3—C4—C23	5.1 (3)	C18—C17—C22—C21	0.0 (4)
C1—S1—C5—C6	−67.9 (2)	C3—C17—C22—C21	179.2 (2)
C7—N3—C6—O1	7.3 (4)	C20—C21—C22—C17	1.1 (4)
C7—N3—C6—C5	−174.7 (2)	N2—C4—C23—C28	44.8 (3)
S1—C5—C6—O1	−13.9 (3)	C3—C4—C23—C28	−136.9 (2)
S1—C5—C6—N3	168.15 (17)	N2—C4—C23—C24	−131.2 (2)
C6—N3—C7—C8	−16.8 (4)	C3—C4—C23—C24	47.1 (3)

C6—N3—C7—C12	162.9 (2)	C28—C23—C24—C25	−1.1 (4)
C12—C7—C8—C9	−1.1 (4)	C4—C23—C24—C25	174.9 (2)
N3—C7—C8—C9	178.7 (2)	C23—C24—C25—C26	0.8 (4)
C7—C8—C9—C10	0.6 (4)	C24—C25—C26—C27	0.4 (4)
C8—C9—C10—C11	−0.5 (4)	C25—C26—C27—C28	−1.2 (4)
C8—C9—C10—C13	177.3 (2)	C24—C23—C28—C27	0.3 (4)
C9—C10—C11—C12	0.8 (4)	C4—C23—C28—C27	−175.9 (2)
C13—C10—C11—C12	−177.0 (2)	C26—C27—C28—C23	0.9 (4)
C10—C11—C12—C7	−1.2 (4)		

Hydrogen-bond geometry (Å, º)

Cg1, Cg2 and Cg4 are the centroids of the pyridazine (N1/N2/C1–C4), 4-methylphenyl (C7–C12) and phenyl (C23–C28) rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3···O1^{i}	0.87	2.21	3.073 (3)	174
C5—H5*B*···O2^{i}	0.99	2.36	3.220 (4)	144
C11—H11···O2^{ii}	0.95	2.43	3.263 (4)	146
C20—H20···*Cg*4^{iii}	0.95	2.61	3.495 (3)	155
C26—H26···*Cg*1^{iv}	0.95	2.80	3.556 (3)	137
C28—H28···*Cg*2^{v}	0.95	2.66	3.484 (3)	146

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