IUCrData

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

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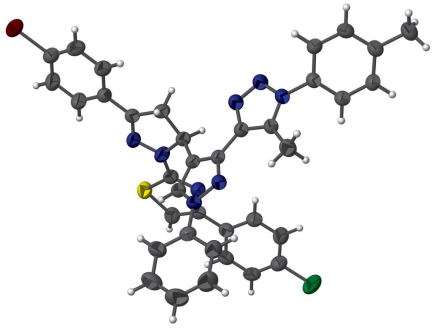
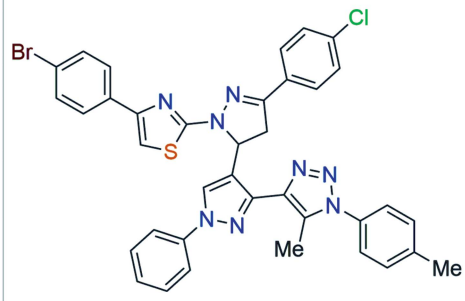
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title compound, $C_{37}H_{28}BrClN_8S$, comprises one molecule. The molecule consists of two ring systems joined by a C—C bond between the dihydropyrazolyl and pyrazolyl rings of the two extended ring systems. The angles between adjacent ring planes of the tolyl–triazolyl–pyrazolyl–phenyl ring system are 48.2 (1), 12.3 (2) and 22.2 (2)°, respectively, with angles of 19.7 (1), 5.6 (2) and 0.9 (2)° between the rings of the chlorophenyl–thiazolyl–dihydropyrazolyl–bromophenyl set. The pyrazolyl and dihydropyrazolyl rings are inclined at 68.3 (1)° to one another. In the crystal, C—H···Cl interactions form chains of molecules parallel to the *b*-axis direction.

3D view



Chemical scheme



Structure description

Various efficient procedures have been reported for the synthesis of pyrazole (Panda & Jena, 2012; Wu *et al.*, 2012) and triazine ring systems (Oudir *et al.*, 2006; Shie & Fang, 2007). Heterocycles containing such moieties show biological activities (Abd El-All *et al.*, 2015; Ansari *et al.*, 2017; El-Barbary *et al.*, 2005). The X-ray crystal structure of a related compound, (*E*)-1-[5-methyl-1-(*p*-tolyl)-1*H*-1,2,3-triazol-4-yl]-3-{3-[5-methyl-1-(*p*-tolyl)-

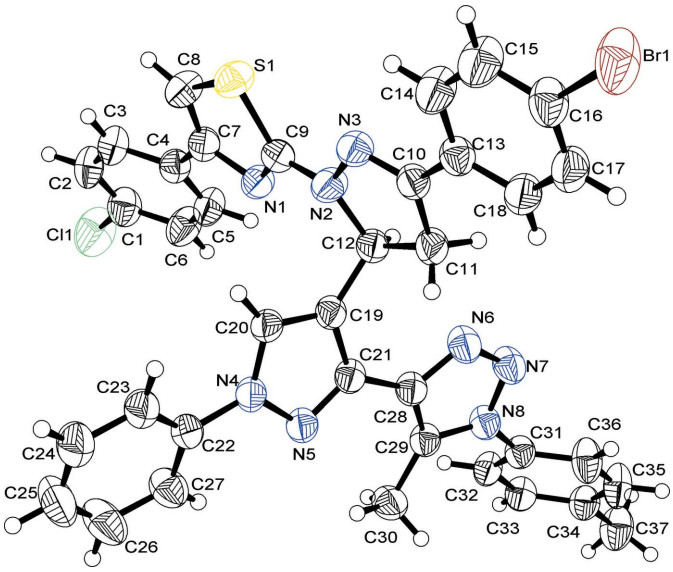


Figure 1
An *ORTEP* representation of the asymmetric unit showing 50% probability ellipsoids.

1*H*-1,2,3-triazol-4-yl]-1-phenyl-1*H*-pyrazol-4-yl}prop-2-en-1-one has been published recently (Abu El-Enin *et al.*, 2017).

The asymmetric unit comprises one molecule of $C_{37}H_{28}BrClN_8S$ (Fig. 1). The molecule consists of two ring systems joined by the C12—C19 bond. The angles between the planes of the tolyl–triazolyl–pyrazolyl–phenyl rings are 48.2 (1), 12.3 (2) and 22.2 (2)°, while those between the planes of the chlorophenyl–thiazolyl–dihydropyrazolyl–bromophenyl rings are 19.7 (1), 5.6 (2) and 0.9 (2)°, respectively. The planes of the pyrazolyl and dihydropyrazolyl rings are inclined at 68.3 (1)°. In the crystal, C5—H5···Cl1 hydrogen bonds form zigzag chains of molecules parallel to the *b*-axis direction (Fig. 2, Table 1).

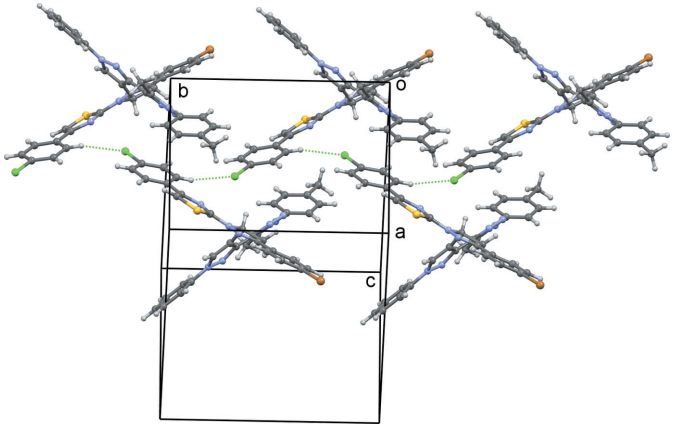


Figure 2
A segment of the crystal structure showing C—H···Cl contacts as dashed lines.

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···Cl1^{i}	0.93	2.89	3.778 (3)	161

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{37}H_{28}BrClN_8S$
M_r	732.09
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	296
a, b, c (Å)	10.4422 (3), 13.3065 (3), 24.0683 (8)
β (°)	90.181 (3)
V (Å^3)	3344.25 (17)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	3.32
Crystal size (mm)	0.49 × 0.09 × 0.05
Data collection	
Diffractometer	Rigaku Oxford Diffraction SuperNova, Dual, Cu at zero, Atlas
Absorption correction	Gaussian (*CrysAlis PRO*; Rigaku OD, 2015)
T_{min}, T_{max}	0.949, 0.992
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	23807, 6739, 5579
R_{int}	0.034
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.624
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.047, 0.138, 1.05
No. of reflections	6739
No. of parameters	435
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.77, −1.04

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SHELXS97* (Sheldrick, 2008), *SHELXL2018* (Sheldrick, 2015), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012) and *CHEMDRAW Ultra* (Cambridge Soft, 2001).

Synthesis and crystallization

The title compound was synthesized based on a literature procedure (Abdel-Wahab *et al.*, 2017) by the reaction of a mixture of equimolar quantities of 3-(4-chlorophenyl)-5-(3-(5-methyl-1-(4-methylphenyl)-1*H*-1,2,3-triazol-4-yl)-1-phenyl-1*H*-pyrazol-4-yl)-4,5-dihydro-1*H*-pyrazole-1-carbothioamide and 2-bromo-1-phenylethanone in refluxing dry ethanol for 2 h. The solid obtained on cooling was collected by filtration, washed with ethanol, dried and recrystallized from dimethylformamide to give yellow crystals (83%), m.p. 279–281°C (lit. m.p. 279–281°C; Abdel-Wahab *et al.*, 2017). The spectroscopic data for the title compound are consistent with those reported (Abdel-Wahab *et al.*, 2017).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Funding information

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full crystallographic data

IUCrData (2018). **3**, x180443 [https://doi.org/10.1107/S2414314618004431]

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

Crystal data

$C_{37}H_{28}BrClN_8S$
M_r = 732.09
Monoclinic, $P2_1/n$
a = 10.4422 (3) Å
b = 13.3065 (3) Å
c = 24.0683 (8) Å
β = 90.181 (3)°
V = 3344.25 (17) Å^3
Z = 4
$F(000)$ = 1496
D_x = 1.454 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 9285 reflections
θ = 3.7–74.2°
μ = 3.32 mm^{-1}
T = 296 K
Needle, yellow
0.49 × 0.09 × 0.05 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} = 0.949, T_{max} = 0.992
23807 measured reflections
6739 independent reflections
5579 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 74.3°, θ_{min} = 3.7°
h = −9→13
k = −16→16
l = −29→28

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.138
S = 1.05
6739 reflections
435 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.065P)^2 + 1.9503P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.77 e Å^{-3}
$\Delta\rho_{min}$ = −1.04 e Å^{-3}

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.2922 (3)	1.1211 (2)	0.21922 (13)	0.0619 (7)
C2	0.3757 (3)	1.1642 (2)	0.18276 (14)	0.0612 (7)
H2	0.369306	1.232184	0.174323	0.073*
C3	0.4700 (3)	1.1059 (2)	0.15841 (13)	0.0558 (6)
H3	0.526327	1.134866	0.133223	0.067*
C4	0.4811 (2)	1.00435 (19)	0.17131 (10)	0.0464 (5)
C5	0.3936 (3)	0.9633 (2)	0.20794 (12)	0.0567 (6)
H5	0.399123	0.895383	0.216661	0.068*
C6	0.2986 (3)	1.0204 (2)	0.23182 (14)	0.0660 (8)
H6	0.239932	0.991458	0.256005	0.079*
C7	0.5829 (2)	0.94164 (18)	0.14708 (10)	0.0458 (5)
C8	0.6520 (3)	0.9630 (2)	0.10122 (11)	0.0552 (6)
H8	0.641481	1.020598	0.079785	0.066*
C9	0.7074 (2)	0.80843 (18)	0.14708 (10)	0.0453 (5)
C10	0.8801 (2)	0.58992 (18)	0.15202 (10)	0.0438 (5)
C11	0.8067 (3)	0.56615 (19)	0.20398 (11)	0.0515 (6)
H11A	0.863850	0.556163	0.235335	0.062*
H11B	0.754168	0.506626	0.199149	0.062*
C12	0.7233 (2)	0.66059 (18)	0.21193 (9)	0.0450 (5)
H12	0.632306	0.643696	0.208392	0.054*
C13	0.9737 (2)	0.52266 (19)	0.12667 (10)	0.0465 (5)
C14	1.0370 (3)	0.5501 (2)	0.07788 (13)	0.0626 (7)
H14	1.020128	0.612167	0.061638	0.075*
C15	1.1241 (3)	0.4862 (2)	0.05370 (14)	0.0696 (8)
H15	1.165783	0.504754	0.021184	0.084*
C16	1.1491 (3)	0.3944 (2)	0.07801 (13)	0.0590 (7)
C17	1.0884 (3)	0.3645 (2)	0.12567 (13)	0.0615 (7)
H17	1.105771	0.302244	0.141528	0.074*
C18	1.0001 (3)	0.4295 (2)	0.14975 (11)	0.0556 (6)
H18	0.957969	0.410073	0.181989	0.067*
C19	0.7488 (2)	0.71190 (17)	0.26631 (9)	0.0410 (5)
C20	0.8273 (2)	0.79145 (17)	0.27590 (9)	0.0427 (5)
H20	0.872623	0.827373	0.249274	0.051*
C21	0.7027 (2)	0.68410 (17)	0.31975 (10)	0.0416 (5)
C22	0.8922 (2)	0.88705 (18)	0.36012 (10)	0.0445 (5)
C23	0.9970 (3)	0.9333 (2)	0.33606 (11)	0.0555 (6)
H23	1.027775	0.911261	0.301957	0.067*
C24	1.0554 (3)	1.0124 (2)	0.36307 (14)	0.0705 (8)
H24	1.125462	1.044056	0.346990	0.085*

C25	1.0108 (4)	1.0445 (3)	0.41342 (16)	0.0832 (10)
H25	1.050677	1.097814	0.431482	0.100*
C26	0.9069 (4)	0.9979 (3)	0.43743 (15)	0.0786 (10)
H26	0.876911	1.020124	0.471628	0.094*
C27	0.8470 (3)	0.9186 (2)	0.41125 (12)	0.0589 (7)
H27	0.777388	0.886771	0.427646	0.071*
C28	0.6135 (2)	0.60317 (18)	0.33277 (10)	0.0435 (5)
C29	0.5439 (2)	0.58454 (17)	0.38029 (10)	0.0425 (5)
C30	0.5483 (3)	0.6320 (2)	0.43635 (10)	0.0547 (6)
H30A	0.475266	0.674961	0.440903	0.082*
H30B	0.625283	0.670933	0.439922	0.082*
H30C	0.547254	0.580589	0.464343	0.082*
C31	0.3757 (2)	0.45259 (18)	0.39841 (10)	0.0441 (5)
C32	0.2830 (2)	0.50835 (18)	0.42458 (10)	0.0474 (5)
H32	0.284781	0.578157	0.422796	0.057*
C33	0.1872 (2)	0.4598 (2)	0.45361 (11)	0.0493 (5)
H33	0.125172	0.497936	0.471547	0.059*
C34	0.1808 (2)	0.3566 (2)	0.45674 (11)	0.0500 (6)
C35	0.2747 (3)	0.3022 (2)	0.42921 (14)	0.0627 (7)
H35	0.271692	0.232421	0.430176	0.075*
C36	0.3726 (3)	0.3487 (2)	0.40040 (14)	0.0604 (7)
H36	0.435162	0.310790	0.382691	0.072*
C37	0.0747 (3)	0.3056 (2)	0.48799 (15)	0.0703 (8)
H37A	0.007207	0.287989	0.462655	0.105*
H37B	0.042087	0.350380	0.515841	0.105*
H37C	0.107183	0.245922	0.505456	0.105*
N1	0.6142 (2)	0.85150 (15)	0.17330 (8)	0.0461 (4)
N2	0.7650 (2)	0.72265 (16)	0.16456 (9)	0.0504 (5)
N3	0.8545 (2)	0.67696 (16)	0.13134 (8)	0.0468 (4)
N4	0.8275 (2)	0.80893 (14)	0.33154 (8)	0.0433 (4)
N5	0.75076 (19)	0.74371 (15)	0.35922 (8)	0.0443 (4)
N6	0.5845 (2)	0.53162 (17)	0.29427 (9)	0.0522 (5)
N7	0.4991 (2)	0.47018 (17)	0.31457 (9)	0.0536 (5)
N8	0.47323 (19)	0.50237 (15)	0.36707 (8)	0.0453 (4)
Cl1	0.17330 (11)	1.19476 (7)	0.25039 (5)	0.0961 (3)
S1	0.76202 (6)	0.86975 (5)	0.08757 (3)	0.05486 (18)
Br1	1.26903 (4)	0.30625 (3)	0.04415 (2)	0.08860 (17)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0619 (16)	0.0500 (15)	0.0737 (18)	0.0087 (12)	0.0066 (14)	−0.0036 (13)
C2	0.0657 (17)	0.0354 (12)	0.083 (2)	0.0016 (12)	0.0036 (14)	0.0015 (12)
C3	0.0552 (14)	0.0433 (13)	0.0691 (17)	−0.0054 (11)	0.0038 (12)	0.0064 (12)
C4	0.0452 (12)	0.0429 (12)	0.0510 (13)	−0.0020 (10)	−0.0021 (10)	0.0009 (10)
C5	0.0623 (15)	0.0407 (13)	0.0672 (16)	0.0030 (11)	0.0114 (13)	0.0078 (12)
C6	0.0705 (18)	0.0552 (16)	0.0724 (18)	0.0061 (14)	0.0232 (15)	0.0111 (14)
C7	0.0467 (12)	0.0412 (12)	0.0494 (12)	−0.0016 (10)	−0.0015 (10)	0.0012 (10)

C8	0.0568 (14)	0.0532 (15)	0.0556 (14)	0.0047 (12)	0.0062 (11)	0.0125 (12)
C9	0.0513 (13)	0.0435 (12)	0.0412 (11)	−0.0003 (10)	0.0021 (10)	−0.0023 (9)
C10	0.0475 (12)	0.0399 (12)	0.0440 (12)	−0.0023 (9)	0.0046 (9)	−0.0036 (9)
C11	0.0688 (16)	0.0384 (12)	0.0475 (13)	0.0005 (11)	0.0139 (11)	−0.0035 (10)
C12	0.0523 (13)	0.0412 (12)	0.0416 (12)	−0.0014 (10)	0.0083 (10)	−0.0024 (9)
C13	0.0464 (12)	0.0433 (12)	0.0498 (13)	−0.0011 (10)	0.0064 (10)	−0.0044 (10)
C14	0.0671 (17)	0.0491 (15)	0.0716 (18)	0.0078 (13)	0.0241 (14)	0.0082 (13)
C15	0.0724 (19)	0.0587 (17)	0.078 (2)	0.0071 (14)	0.0353 (16)	0.0085 (15)
C16	0.0582 (15)	0.0461 (14)	0.0728 (18)	0.0045 (12)	0.0136 (13)	−0.0061 (12)
C17	0.0785 (19)	0.0419 (13)	0.0642 (17)	0.0072 (13)	0.0113 (14)	0.0009 (12)
C18	0.0691 (16)	0.0445 (13)	0.0533 (14)	0.0013 (12)	0.0131 (12)	0.0009 (11)
C19	0.0461 (11)	0.0360 (11)	0.0411 (11)	0.0010 (9)	0.0078 (9)	−0.0024 (9)
C20	0.0514 (12)	0.0387 (11)	0.0381 (11)	−0.0014 (9)	0.0085 (9)	0.0003 (9)
C21	0.0447 (11)	0.0369 (11)	0.0433 (11)	0.0009 (9)	0.0101 (9)	−0.0012 (9)
C22	0.0520 (13)	0.0375 (11)	0.0440 (12)	0.0015 (10)	0.0004 (10)	−0.0030 (9)
C23	0.0664 (16)	0.0481 (14)	0.0520 (14)	−0.0115 (12)	0.0054 (12)	−0.0008 (11)
C24	0.081 (2)	0.0608 (18)	0.0693 (19)	−0.0235 (16)	0.0040 (15)	−0.0008 (14)
C25	0.094 (2)	0.068 (2)	0.087 (2)	−0.0258 (19)	−0.0005 (19)	−0.0274 (18)
C26	0.083 (2)	0.085 (2)	0.0681 (19)	−0.0104 (18)	0.0112 (16)	−0.0351 (17)
C27	0.0592 (15)	0.0628 (17)	0.0547 (15)	−0.0047 (13)	0.0075 (12)	−0.0134 (13)
C28	0.0459 (12)	0.0405 (11)	0.0440 (12)	−0.0009 (9)	0.0082 (9)	−0.0023 (9)
C29	0.0428 (11)	0.0400 (11)	0.0449 (12)	−0.0015 (9)	0.0069 (9)	0.0000 (9)
C30	0.0606 (15)	0.0587 (15)	0.0450 (13)	−0.0109 (12)	0.0078 (11)	−0.0034 (11)
C31	0.0434 (12)	0.0421 (12)	0.0468 (12)	−0.0043 (9)	0.0063 (9)	0.0002 (10)
C32	0.0517 (13)	0.0373 (11)	0.0531 (13)	0.0000 (10)	0.0082 (10)	0.0036 (10)
C33	0.0466 (12)	0.0479 (13)	0.0534 (13)	0.0023 (10)	0.0112 (10)	−0.0006 (10)
C34	0.0469 (12)	0.0463 (13)	0.0567 (14)	−0.0050 (10)	0.0055 (10)	0.0023 (11)
C35	0.0606 (16)	0.0371 (13)	0.091 (2)	−0.0047 (11)	0.0197 (15)	−0.0009 (13)
C36	0.0554 (15)	0.0417 (13)	0.084 (2)	−0.0008 (11)	0.0233 (14)	−0.0084 (13)
C37	0.0640 (18)	0.0562 (17)	0.091 (2)	−0.0112 (13)	0.0252 (16)	0.0063 (15)
N1	0.0499 (11)	0.0430 (10)	0.0455 (10)	0.0022 (9)	0.0051 (8)	0.0028 (8)
N2	0.0616 (12)	0.0456 (11)	0.0441 (10)	0.0101 (9)	0.0126 (9)	0.0028 (9)
N3	0.0491 (11)	0.0475 (11)	0.0440 (10)	0.0032 (9)	0.0098 (8)	0.0001 (8)
N4	0.0515 (11)	0.0358 (10)	0.0426 (10)	−0.0034 (8)	0.0086 (8)	−0.0019 (7)
N5	0.0495 (10)	0.0406 (10)	0.0429 (10)	−0.0037 (8)	0.0103 (8)	−0.0016 (8)
N6	0.0566 (12)	0.0490 (12)	0.0512 (11)	−0.0091 (9)	0.0163 (9)	−0.0078 (9)
N7	0.0583 (12)	0.0495 (12)	0.0531 (12)	−0.0103 (10)	0.0159 (10)	−0.0101 (9)
N8	0.0462 (10)	0.0427 (10)	0.0471 (11)	−0.0057 (8)	0.0100 (8)	−0.0026 (8)
Cl1	0.1044 (7)	0.0663 (5)	0.1178 (8)	0.0307 (5)	0.0396 (6)	0.0029 (5)
S1	0.0563 (4)	0.0581 (4)	0.0502 (3)	0.0051 (3)	0.0110 (3)	0.0087 (3)
Br1	0.0960 (3)	0.0521 (2)	0.1181 (3)	0.01555 (17)	0.0517 (2)	−0.00092 (18)

Geometric parameters (Å, º)

C1—C2	1.365 (4)	C20—H20	0.9300
C1—C6	1.376 (4)	C21—N5	1.334 (3)
C1—Cl1	1.752 (3)	C21—C28	1.459 (3)
C2—C3	1.385 (4)	C22—C27	1.384 (4)

C2—H2	0.9300	C22—C23	1.385 (4)
C3—C4	1.391 (4)	C22—N4	1.417 (3)
C3—H3	0.9300	C23—C24	1.377 (4)
C4—C5	1.384 (4)	C23—H23	0.9300
C4—C7	1.474 (3)	C24—C25	1.368 (5)
C5—C6	1.376 (4)	C24—H24	0.9300
C5—H5	0.9300	C25—C26	1.379 (5)
C6—H6	0.9300	C25—H25	0.9300
C7—C8	1.350 (4)	C26—C27	1.378 (4)
C7—N1	1.394 (3)	C26—H26	0.9300
C8—S1	1.724 (3)	C27—H27	0.9300
C8—H8	0.9300	C28—N6	1.362 (3)
C9—N1	1.295 (3)	C28—C29	1.380 (3)
C9—N2	1.357 (3)	C29—N8	1.356 (3)
C9—S1	1.746 (2)	C29—C30	1.490 (3)
C10—N3	1.288 (3)	C30—H30A	0.9600
C10—C13	1.460 (3)	C30—H30B	0.9600
C10—C11	1.503 (3)	C30—H30C	0.9600
C11—C12	1.541 (3)	C31—C32	1.374 (3)
C11—H11A	0.9700	C31—C36	1.384 (4)
C11—H11B	0.9700	C31—N8	1.431 (3)
C12—N2	1.475 (3)	C32—C33	1.383 (3)
C12—C19	1.499 (3)	C32—H32	0.9300
C12—H12	0.9800	C33—C34	1.376 (4)
C13—C18	1.385 (4)	C33—H33	0.9300
C13—C14	1.398 (4)	C34—C35	1.389 (4)
C14—C15	1.376 (4)	C34—C37	1.502 (4)
C14—H14	0.9300	C35—C36	1.383 (4)
C15—C16	1.379 (4)	C35—H35	0.9300
C15—H15	0.9300	C36—H36	0.9300
C16—C17	1.371 (4)	C37—H37A	0.9600
C16—Br1	1.902 (3)	C37—H37B	0.9600
C17—C18	1.392 (4)	C37—H37C	0.9600
C17—H17	0.9300	N2—N3	1.374 (3)
C18—H18	0.9300	N4—N5	1.357 (3)
C19—C20	1.358 (3)	N6—N7	1.306 (3)
C19—C21	1.424 (3)	N7—N8	1.362 (3)
C20—N4	1.359 (3)		

C2—C1—C6	121.3 (3)	C27—C22—C23	120.6 (2)
C2—C1—Cl1	119.7 (2)	C27—C22—N4	119.4 (2)
C6—C1—Cl1	119.0 (2)	C23—C22—N4	120.0 (2)
C1—C2—C3	119.6 (3)	C24—C23—C22	119.4 (3)
C1—C2—H2	120.2	C24—C23—H23	120.3
C3—C2—H2	120.2	C22—C23—H23	120.3
C2—C3—C4	120.6 (3)	C25—C24—C23	120.3 (3)
C2—C3—H3	119.7	C25—C24—H24	119.8
C4—C3—H3	119.7	C23—C24—H24	119.8

C5—C4—C3	118.1 (2)	C24—C25—C26	120.1 (3)
C5—C4—C7	120.5 (2)	C24—C25—H25	120.0
C3—C4—C7	121.4 (2)	C26—C25—H25	120.0
C6—C5—C4	121.8 (3)	C27—C26—C25	120.6 (3)
C6—C5—H5	119.1	C27—C26—H26	119.7
C4—C5—H5	119.1	C25—C26—H26	119.7
C1—C6—C5	118.7 (3)	C26—C27—C22	118.9 (3)
C1—C6—H6	120.6	C26—C27—H27	120.6
C5—C6—H6	120.6	C22—C27—H27	120.6
C8—C7—N1	115.2 (2)	N6—C28—C29	108.8 (2)
C8—C7—C4	126.3 (2)	N6—C28—C21	120.7 (2)
N1—C7—C4	118.5 (2)	C29—C28—C21	130.5 (2)
C7—C8—S1	111.2 (2)	N8—C29—C28	103.8 (2)
C7—C8—H8	124.4	N8—C29—C30	124.7 (2)
S1—C8—H8	124.4	C28—C29—C30	131.3 (2)
N1—C9—N2	123.7 (2)	C29—C30—H30A	109.5
N1—C9—S1	116.16 (18)	C29—C30—H30B	109.5
N2—C9—S1	120.11 (19)	H30A—C30—H30B	109.5
N3—C10—C13	121.8 (2)	C29—C30—H30C	109.5
N3—C10—C11	113.9 (2)	H30A—C30—H30C	109.5
C13—C10—C11	124.2 (2)	H30B—C30—H30C	109.5
C10—C11—C12	102.8 (2)	C32—C31—C36	120.5 (2)
C10—C11—H11A	111.2	C32—C31—N8	119.7 (2)
C12—C11—H11A	111.2	C36—C31—N8	119.8 (2)
C10—C11—H11B	111.2	C31—C32—C33	119.4 (2)
C12—C11—H11B	111.2	C31—C32—H32	120.3
H11A—C11—H11B	109.1	C33—C32—H32	120.3
N2—C12—C19	111.6 (2)	C34—C33—C32	121.9 (2)
N2—C12—C11	101.09 (18)	C34—C33—H33	119.0
C19—C12—C11	112.4 (2)	C32—C33—H33	119.0
N2—C12—H12	110.5	C33—C34—C35	117.3 (2)
C19—C12—H12	110.5	C33—C34—C37	120.9 (2)
C11—C12—H12	110.5	C35—C34—C37	121.8 (2)
C18—C13—C14	118.5 (2)	C36—C35—C34	122.1 (2)
C18—C13—C10	120.9 (2)	C36—C35—H35	119.0
C14—C13—C10	120.6 (2)	C34—C35—H35	119.0
C15—C14—C13	120.6 (3)	C35—C36—C31	118.8 (2)
C15—C14—H14	119.7	C35—C36—H36	120.6
C13—C14—H14	119.7	C31—C36—H36	120.6
C14—C15—C16	119.5 (3)	C34—C37—H37A	109.5
C14—C15—H15	120.2	C34—C37—H37B	109.5
C16—C15—H15	120.2	H37A—C37—H37B	109.5
C17—C16—C15	121.6 (3)	C34—C37—H37C	109.5
C17—C16—Br1	119.1 (2)	H37A—C37—H37C	109.5
C15—C16—Br1	119.2 (2)	H37B—C37—H37C	109.5
C16—C17—C18	118.4 (3)	C9—N1—C7	109.6 (2)
C16—C17—H17	120.8	C9—N2—N3	119.6 (2)
C18—C17—H17	120.8	C9—N2—C12	125.4 (2)

C13—C18—C17	121.4 (3)	N3—N2—C12	113.92 (19)
C13—C18—H18	119.3	C10—N3—N2	108.3 (2)
C17—C18—H18	119.3	N5—N4—C20	112.04 (19)
C20—C19—C21	104.8 (2)	N5—N4—C22	120.81 (19)
C20—C19—C12	127.5 (2)	C20—N4—C22	127.1 (2)
C21—C19—C12	127.6 (2)	C21—N5—N4	104.58 (18)
C19—C20—N4	107.4 (2)	N7—N6—C28	109.5 (2)
C19—C20—H20	126.3	N6—N7—N8	106.73 (19)
N4—C20—H20	126.3	C29—N8—N7	111.21 (19)
N5—C21—C19	111.2 (2)	C29—N8—C31	129.6 (2)
N5—C21—C28	121.7 (2)	N7—N8—C31	119.12 (19)
C19—C21—C28	127.2 (2)	C8—S1—C9	87.72 (12)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···Cl1^{i}	0.93	2.89	3.778 (3)	161

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