IUCrData

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4-(4-Bromophenyl)-2-(3-(4-bromophenyl)-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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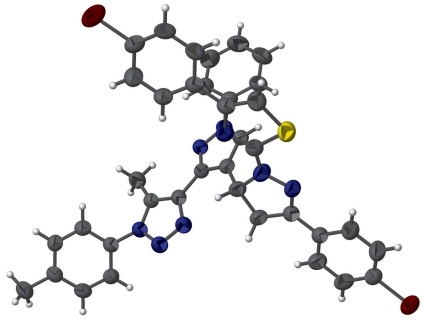
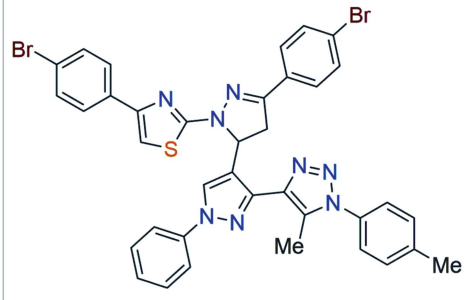
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{37}H_{28}Br_2N_8S$, the dihedral angles between the planes of tolyl–triazolyl–pyrazolyl–phenyl rings are 47.5 (1), 11.4 (2) and 22.4 (2)°, respectively, and the angles between the bromophenyl–thiazolyl–dihydropyrazolyl–bromophenyl rings are 16.0 (2), 5.1 (2) and 0.8 (2)°, respectively. The dihedral angle between the planes of the pyrazolyl and dihydropyrazolyl rings is 67.7 (1)°. In the crystal, weak C—H···Br interactions form chains of molecules propagating in the [010] direction.

3D view



Chemical scheme



Structure description

Several synthetic procedures have been reported for the synthesis of pyrazole, thiazole and triazole-containing heterocycles (Assarzadeh *et al.*, 2014; Hassan *et al.*, 2014; Sarigol *et al.*, 2015). Compounds with pyrazolylthiazole and pyrazolyltriazole ring systems show a variety of biological activities (Dawood *et al.*, 2013; Dayakar *et al.*, 2017; Gomha *et al.*, 2016). The X-ray crystal structure for a related compound has been recently published (Abu El-Enin *et al.*, 2017).

The asymmetric unit comprises one molecule of $C_{37}H_{28}Br_2N_8S$ (Fig. 1). The molecule can be considered as two sets of rings linked by the C10—C19 bond. The dihedral angles

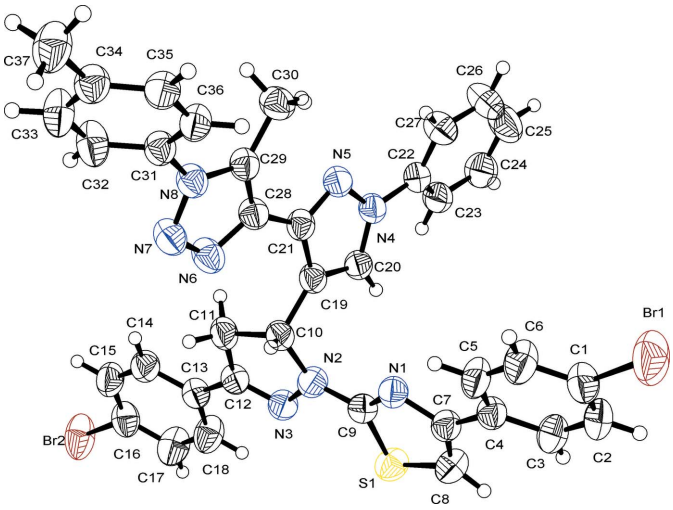


Figure 1
The title compound showing 50% displacement ellipsoids.

between the planes of tolyl–triazolyl–pyrazolyl–phenyl rings are 47.5 (1), 11.4 (2) and 22.4 (2)°, respectively, in the first set. In the second set, the dihedral angles between the bromophenyl–thiazolyl–dihydropyrazolyl–bromophenyl rings are 16.0 (2), 5.1 (2) and 0.8 (2)°, respectively. The dihedral angle between the planes of the pyrazolyl and dihydropyrazolyl rings is 67.7 (1)°. In the crystal, weak C—H···Br interactions form chains of molecules parallel to the *b*-axis direction (Table 1, Fig. 2) with adjacent molecules in the chain related by the 2_1 screw axis.

Synthesis and crystallization

The title compound was synthesized using a literature procedure (Abdel-Wahab *et al.*, 2017) and colourless needles were recrystallized from dimethylformamide solution.

Refinement

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

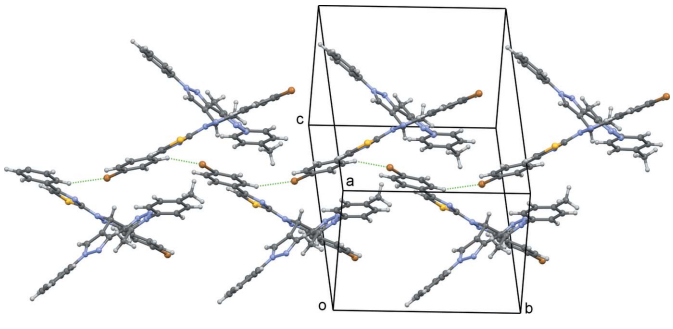


Figure 2
A segment of the crystal structure showing C—H···Br contacts.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···Br1^{i}	0.93	2.87	3.741 (3)	157

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{37}H_{28}Br_2N_8S$
M_r	776.55
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	293
a, *b*, *c* (Å)	10.3624 (2), 13.5082 (3), 24.0262 (6)
β (°)	90.457 (2)
V (Å^3)	3363.02 (13)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	3.96
Crystal size (mm)	0.24 × 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}	0.971, 0.995
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	24126, 6772, 5247
R_{int}	0.037
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.052, 0.162, 1.05
No. of reflections	6772
No. of parameters	435
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.06, −1.26

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

Funding information

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full crystallographic data

IUCrData (2018). **3**, x180449 [https://doi.org/10.1107/S2414314618004492]

4-(4-Bromophenyl)-2-(3-(4-bromophenyl)-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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Crystal data

$C_{37}H_{28}Br_2N_8S$
M_r = 776.55
Monoclinic, $P2_1/n$
a = 10.3624 (2) Å
b = 13.5082 (3) Å
c = 24.0262 (6) Å
β = 90.457 (2)°
V = 3363.02 (13) Å^3
Z = 4
$F(000)$ = 1568
D_x = 1.534 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 7424 reflections
θ = 3.6–74.1°
μ = 3.96 mm^{-1}
T = 293 K
Needle, colourless
0.24 × 0.09 × 0.05 mm

Data collection

Rigaku Oxford Diffraction SuperNova, Dual, Cu at zero, Atlas diffractometer
ω scans
Absorption correction: gaussian (CrysAlisPro; Rigaku OD, 2015)
T_{min} = 0.971, T_{max} = 0.995
24126 measured reflections
6772 independent reflections
5247 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 74.4°, θ_{min} = 3.7°
h = −11→12
k = −16→16
l = −29→26

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.162
S = 1.05
6772 reflections
435 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0831P)^2 + 2.1716P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.06 e Å^{-3}
$\Delta\rho_{min}$ = −1.26 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.

Refinement. All hydrogen atoms were placed in calculated positions and refined using a riding model. Aromatic C—H distances were set to 0.93 Å and their U(iso) set to 1.2 times the U_{eq} for the atoms to which they are bonded. Methine C—H distances were set to 0.98 Å and their U(iso) set to 1.2 times the U_{eq} for the atoms to which they are bonded. Methylene C—H distances were set to 0.97 Å and their U(iso) set to 1.2 times the U_{eq} for the atoms to which they are bonded. Methyl groups were allowed to rotate about the C—C bond and C—H distances were set to 0.96 Å with U(iso) set to 1.5 times the U_{eq} for the C atoms to which they are bonded.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.6973 (4)	0.3731 (3)	0.28057 (17)	0.0651 (9)
C2	0.6176 (4)	0.3335 (3)	0.31946 (17)	0.0641 (9)
H2	0.625004	0.267133	0.329169	0.077*
C3	0.5256 (3)	0.3922 (2)	0.34446 (16)	0.0603 (8)
H3	0.471807	0.365079	0.371241	0.072*
C4	0.5127 (3)	0.4917 (2)	0.32994 (14)	0.0508 (7)
C5	0.5965 (4)	0.5294 (3)	0.29070 (16)	0.0637 (9)
H5	0.589857	0.595704	0.280653	0.076*
C6	0.6894 (4)	0.4714 (3)	0.26610 (18)	0.0719 (10)
H6	0.745692	0.498252	0.240208	0.086*
C7	0.4122 (3)	0.5552 (2)	0.35431 (13)	0.0506 (7)
C8	0.3420 (3)	0.5346 (3)	0.40002 (15)	0.0610 (8)
H8	0.350841	0.477459	0.421294	0.073*
C9	0.2914 (3)	0.6884 (2)	0.35436 (13)	0.0508 (7)
C10	0.2794 (3)	0.8355 (2)	0.28957 (12)	0.0511 (7)
H10	0.371431	0.850916	0.293508	0.061*
C11	0.1968 (4)	0.9295 (2)	0.29769 (14)	0.0572 (8)
H11A	0.250633	0.987460	0.303169	0.069*
H11B	0.139881	0.940552	0.266035	0.069*
C12	0.1214 (3)	0.9060 (2)	0.34918 (13)	0.0494 (7)
C13	0.0284 (3)	0.9733 (2)	0.37463 (13)	0.0511 (7)
C14	0.0054 (4)	1.0665 (3)	0.35213 (15)	0.0623 (8)
H14	0.049303	1.085800	0.320319	0.075*
C15	−0.0819 (4)	1.1312 (3)	0.37621 (17)	0.0666 (9)
H15	−0.097030	1.193332	0.360759	0.080*
C16	−0.1455 (4)	1.1017 (3)	0.42334 (17)	0.0640 (9)
C17	−0.1242 (4)	1.0100 (3)	0.44684 (19)	0.0750 (11)
H17	−0.168056	0.991438	0.478790	0.090*
C18	−0.0376 (4)	0.9463 (3)	0.42278 (18)	0.0697 (10)
H18	−0.022776	0.884545	0.438717	0.084*
C19	0.2525 (3)	0.7858 (2)	0.23482 (12)	0.0464 (6)
C20	0.1731 (3)	0.7073 (2)	0.22478 (13)	0.0489 (7)
H20	0.127363	0.671684	0.251249	0.059*
C21	0.2988 (3)	0.8134 (2)	0.18174 (13)	0.0467 (6)

C22	0.1075 (3)	0.6137 (2)	0.13990 (13)	0.0499 (7)
C23	0.0020 (4)	0.5679 (3)	0.16363 (14)	0.0592 (8)
H23	−0.029384	0.589652	0.197666	0.071*
C24	−0.0560 (4)	0.4900 (3)	0.13649 (18)	0.0737 (10)
H24	−0.126517	0.458539	0.152406	0.088*
C25	−0.0108 (5)	0.4585 (3)	0.0863 (2)	0.0858 (13)
H25	−0.050553	0.405750	0.068145	0.103*
C26	0.0935 (5)	0.5048 (4)	0.06260 (18)	0.0814 (12)
H26	0.123955	0.483029	0.028413	0.098*
C27	0.1535 (4)	0.5832 (3)	0.08898 (15)	0.0629 (8)
H27	0.223532	0.614806	0.072782	0.075*
C28	0.3889 (3)	0.8933 (2)	0.16866 (13)	0.0484 (6)
C29	0.4572 (3)	0.9133 (2)	0.12084 (13)	0.0478 (6)
C30	0.4513 (4)	0.8675 (3)	0.06460 (14)	0.0604 (8)
H30A	0.450006	0.918545	0.036809	0.091*
H30B	0.374530	0.828110	0.061299	0.091*
H30C	0.525694	0.826229	0.059384	0.091*
C31	0.6254 (3)	1.0440 (2)	0.10339 (13)	0.0491 (7)
C32	0.6289 (4)	1.1467 (3)	0.10291 (18)	0.0670 (9)
H32	0.566534	1.183148	0.121488	0.080*
C33	0.7265 (4)	1.1939 (3)	0.07445 (19)	0.0688 (10)
H33	0.729841	1.262673	0.074715	0.083*
C34	0.8197 (3)	1.1416 (3)	0.04547 (15)	0.0561 (7)
C35	0.8135 (3)	1.0398 (3)	0.04709 (14)	0.0549 (7)
H35	0.875406	1.003122	0.028335	0.066*
C36	0.7179 (3)	0.9905 (2)	0.07575 (14)	0.0535 (7)
H36	0.716152	0.921723	0.076350	0.064*
C37	0.9254 (4)	1.1942 (3)	0.0147 (2)	0.0761 (11)
H37A	0.959317	1.151361	−0.013472	0.114*
H37B	0.993050	1.211934	0.040364	0.114*
H37C	0.891225	1.253011	−0.002358	0.114*
N1	0.3837 (3)	0.6446 (2)	0.32804 (11)	0.0524 (6)
N2	0.2349 (3)	0.7741 (2)	0.33681 (11)	0.0565 (6)
N3	0.1453 (3)	0.8199 (2)	0.36979 (11)	0.0523 (6)
N4	0.1729 (3)	0.69057 (18)	0.16912 (11)	0.0493 (6)
N5	0.2502 (3)	0.75534 (19)	0.14154 (10)	0.0494 (6)
N6	0.4192 (3)	0.9628 (2)	0.20785 (12)	0.0593 (7)
N7	0.5043 (3)	1.0237 (2)	0.18751 (12)	0.0601 (7)
N8	0.5289 (3)	0.9938 (2)	0.13477 (11)	0.0512 (6)
S1	0.23386 (9)	0.62837 (7)	0.41369 (4)	0.0613 (2)
Br1	0.82136 (6)	0.29156 (4)	0.24450 (3)	0.1019 (2)
Br2	−0.26346 (5)	1.19038 (3)	0.45748 (3)	0.0937 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.071 (2)	0.0499 (18)	0.074 (2)	0.0077 (16)	0.0066 (18)	−0.0076 (16)
C2	0.072 (2)	0.0374 (15)	0.083 (2)	−0.0004 (15)	0.0010 (18)	0.0030 (16)

C3	0.0609 (19)	0.0454 (17)	0.075 (2)	−0.0050 (14)	0.0041 (16)	0.0091 (15)
C4	0.0540 (16)	0.0436 (15)	0.0548 (17)	−0.0027 (13)	−0.0007 (13)	−0.0002 (13)
C5	0.074 (2)	0.0402 (16)	0.077 (2)	0.0030 (15)	0.0170 (18)	0.0095 (15)
C6	0.079 (2)	0.054 (2)	0.083 (3)	0.0086 (17)	0.025 (2)	0.0130 (18)
C7	0.0528 (16)	0.0455 (15)	0.0534 (16)	−0.0032 (13)	−0.0014 (13)	0.0021 (13)
C8	0.0598 (19)	0.059 (2)	0.064 (2)	0.0047 (15)	0.0045 (15)	0.0129 (16)
C9	0.0573 (17)	0.0481 (16)	0.0471 (16)	−0.0010 (13)	0.0006 (13)	0.0000 (13)
C10	0.0636 (18)	0.0440 (15)	0.0458 (15)	−0.0014 (13)	0.0064 (13)	−0.0039 (12)
C11	0.072 (2)	0.0435 (16)	0.0559 (18)	0.0006 (14)	0.0141 (15)	−0.0061 (13)
C12	0.0506 (15)	0.0467 (16)	0.0511 (16)	−0.0027 (13)	0.0030 (12)	−0.0041 (13)
C13	0.0513 (16)	0.0478 (16)	0.0543 (16)	−0.0018 (13)	0.0050 (13)	−0.0036 (13)
C14	0.079 (2)	0.0512 (18)	0.0568 (18)	0.0013 (16)	0.0120 (16)	−0.0010 (15)
C15	0.083 (2)	0.0461 (18)	0.071 (2)	0.0080 (16)	0.0106 (19)	0.0006 (16)
C16	0.062 (2)	0.0521 (18)	0.078 (2)	0.0020 (15)	0.0119 (17)	−0.0082 (17)
C17	0.073 (2)	0.067 (2)	0.085 (3)	0.0066 (19)	0.033 (2)	0.009 (2)
C18	0.071 (2)	0.056 (2)	0.083 (2)	0.0093 (17)	0.0233 (19)	0.0087 (18)
C19	0.0507 (15)	0.0411 (14)	0.0474 (15)	0.0025 (12)	0.0070 (12)	−0.0024 (12)
C20	0.0580 (17)	0.0432 (15)	0.0456 (15)	−0.0022 (12)	0.0091 (12)	0.0002 (12)
C21	0.0478 (15)	0.0416 (15)	0.0508 (15)	0.0018 (11)	0.0078 (12)	−0.0006 (12)
C22	0.0572 (17)	0.0418 (15)	0.0508 (16)	−0.0011 (12)	−0.0001 (13)	−0.0023 (12)
C23	0.072 (2)	0.0521 (18)	0.0542 (18)	−0.0113 (15)	0.0042 (15)	−0.0009 (14)
C24	0.086 (3)	0.061 (2)	0.075 (2)	−0.0232 (19)	0.004 (2)	0.0020 (18)
C25	0.101 (3)	0.069 (3)	0.087 (3)	−0.024 (2)	0.000 (2)	−0.026 (2)
C26	0.092 (3)	0.083 (3)	0.069 (2)	−0.009 (2)	0.011 (2)	−0.031 (2)
C27	0.064 (2)	0.066 (2)	0.0593 (19)	−0.0034 (16)	0.0058 (15)	−0.0120 (16)
C28	0.0496 (15)	0.0463 (15)	0.0494 (15)	−0.0028 (12)	0.0071 (12)	−0.0029 (12)
C29	0.0485 (15)	0.0430 (15)	0.0521 (16)	−0.0023 (12)	0.0059 (12)	−0.0021 (12)
C30	0.067 (2)	0.062 (2)	0.0517 (17)	−0.0124 (16)	0.0086 (15)	−0.0056 (15)
C31	0.0498 (15)	0.0452 (15)	0.0525 (16)	−0.0047 (12)	0.0049 (12)	−0.0005 (13)
C32	0.062 (2)	0.0477 (18)	0.092 (3)	−0.0034 (15)	0.0217 (18)	−0.0099 (17)
C33	0.068 (2)	0.0410 (17)	0.098 (3)	−0.0050 (15)	0.017 (2)	−0.0012 (17)
C34	0.0547 (17)	0.0520 (18)	0.0618 (19)	−0.0070 (14)	0.0046 (14)	0.0020 (14)
C35	0.0553 (17)	0.0521 (17)	0.0575 (18)	0.0020 (14)	0.0112 (14)	0.0009 (14)
C36	0.0575 (17)	0.0427 (15)	0.0603 (18)	0.0027 (13)	0.0053 (14)	0.0034 (13)
C37	0.071 (2)	0.059 (2)	0.099 (3)	−0.0102 (17)	0.023 (2)	0.009 (2)
N1	0.0606 (15)	0.0463 (14)	0.0505 (14)	0.0031 (11)	0.0052 (11)	0.0009 (11)
N2	0.0691 (16)	0.0521 (15)	0.0485 (14)	0.0103 (13)	0.0123 (12)	0.0019 (12)
N3	0.0565 (14)	0.0516 (14)	0.0490 (13)	0.0035 (11)	0.0101 (11)	−0.0008 (11)
N4	0.0582 (14)	0.0416 (13)	0.0480 (13)	−0.0037 (10)	0.0057 (11)	−0.0017 (10)
N5	0.0551 (14)	0.0455 (13)	0.0478 (13)	−0.0040 (11)	0.0101 (11)	−0.0017 (11)
N6	0.0642 (16)	0.0563 (16)	0.0576 (15)	−0.0105 (13)	0.0155 (13)	−0.0111 (13)
N7	0.0653 (16)	0.0559 (16)	0.0593 (16)	−0.0120 (13)	0.0146 (13)	−0.0115 (13)
N8	0.0531 (14)	0.0477 (14)	0.0529 (14)	−0.0059 (11)	0.0082 (11)	−0.0039 (11)
S1	0.0628 (5)	0.0643 (5)	0.0571 (5)	0.0053 (4)	0.0110 (4)	0.0088 (4)
Br1	0.1222 (5)	0.0676 (3)	0.1165 (4)	0.0333 (3)	0.0368 (3)	0.0011 (3)
Br2	0.1003 (4)	0.0578 (3)	0.1239 (4)	0.0151 (2)	0.0496 (3)	−0.0028 (2)

Geometric parameters (Å, º)

C1—C2	1.361 (6)	C20—H20	0.9300
C1—C6	1.376 (5)	C21—N5	1.339 (4)
C1—Br1	1.906 (4)	C21—C28	1.463 (4)
C2—C3	1.380 (5)	C22—C27	1.380 (5)
C2—H2	0.9300	C22—C23	1.383 (5)
C3—C4	1.395 (5)	C22—N4	1.422 (4)
C3—H3	0.9300	C23—C24	1.374 (5)
C4—C5	1.384 (5)	C23—H23	0.9300
C4—C7	1.474 (5)	C24—C25	1.365 (6)
C5—C6	1.378 (5)	C24—H24	0.9300
C5—H5	0.9300	C25—C26	1.377 (6)
C6—H6	0.9300	C25—H25	0.9300
C7—C8	1.351 (5)	C26—C27	1.379 (5)
C7—N1	1.394 (4)	C26—H26	0.9300
C8—S1	1.725 (4)	C27—H27	0.9300
C8—H8	0.9300	C28—N6	1.365 (4)
C9—N1	1.294 (4)	C28—C29	1.381 (4)
C9—N2	1.362 (4)	C29—N8	1.358 (4)
C9—S1	1.749 (3)	C29—C30	1.487 (4)
C10—N2	1.482 (4)	C30—H30A	0.9600
C10—C19	1.501 (4)	C30—H30B	0.9600
C10—C11	1.545 (4)	C30—H30C	0.9600
C10—H10	0.9800	C31—C36	1.376 (4)
C11—C12	1.503 (4)	C31—C32	1.387 (5)
C11—H11A	0.9700	C31—N8	1.428 (4)
C11—H11B	0.9700	C32—C33	1.381 (5)
C12—N3	1.286 (4)	C32—H32	0.9300
C12—C13	1.462 (4)	C33—C34	1.388 (5)
C13—C14	1.390 (5)	C33—H33	0.9300
C13—C18	1.397 (5)	C34—C35	1.377 (5)
C14—C15	1.388 (5)	C34—C37	1.505 (5)
C14—H14	0.9300	C35—C36	1.381 (5)
C15—C16	1.374 (5)	C35—H35	0.9300
C15—H15	0.9300	C36—H36	0.9300
C16—C17	1.378 (6)	C37—H37A	0.9600
C16—Br2	1.902 (4)	C37—H37B	0.9600
C17—C18	1.374 (5)	C37—H37C	0.9600
C17—H17	0.9300	N2—N3	1.373 (4)
C18—H18	0.9300	N4—N5	1.362 (4)
C19—C20	1.363 (4)	N6—N7	1.304 (4)
C19—C21	1.416 (4)	N7—N8	1.356 (4)
C20—N4	1.356 (4)		
C2—C1—C6	121.1 (3)	C27—C22—C23	120.8 (3)
C2—C1—Br1	120.1 (3)	C27—C22—N4	119.3 (3)
C6—C1—Br1	118.8 (3)	C23—C22—N4	119.9 (3)

C1—C2—C3	119.9 (3)	C24—C23—C22	119.4 (3)
C1—C2—H2	120.0	C24—C23—H23	120.3
C3—C2—H2	120.0	C22—C23—H23	120.3
C2—C3—C4	120.6 (3)	C25—C24—C23	120.4 (4)
C2—C3—H3	119.7	C25—C24—H24	119.8
C4—C3—H3	119.7	C23—C24—H24	119.8
C5—C4—C3	117.8 (3)	C24—C25—C26	120.0 (4)
C5—C4—C7	120.3 (3)	C24—C25—H25	120.0
C3—C4—C7	121.9 (3)	C26—C25—H25	120.0
C6—C5—C4	121.8 (3)	C25—C26—C27	120.7 (4)
C6—C5—H5	119.1	C25—C26—H26	119.6
C4—C5—H5	119.1	C27—C26—H26	119.6
C1—C6—C5	118.8 (4)	C26—C27—C22	118.6 (4)
C1—C6—H6	120.6	C26—C27—H27	120.7
C5—C6—H6	120.6	C22—C27—H27	120.7
C8—C7—N1	115.6 (3)	N6—C28—C29	108.8 (3)
C8—C7—C4	126.1 (3)	N6—C28—C21	120.2 (3)
N1—C7—C4	118.2 (3)	C29—C28—C21	130.9 (3)
C7—C8—S1	111.0 (3)	N8—C29—C28	103.6 (3)
C7—C8—H8	124.5	N8—C29—C30	125.1 (3)
S1—C8—H8	124.5	C28—C29—C30	131.1 (3)
N1—C9—N2	123.7 (3)	C29—C30—H30A	109.5
N1—C9—S1	116.4 (2)	C29—C30—H30B	109.5
N2—C9—S1	119.9 (2)	H30A—C30—H30B	109.5
N2—C10—C19	111.3 (3)	C29—C30—H30C	109.5
N2—C10—C11	100.8 (2)	H30A—C30—H30C	109.5
C19—C10—C11	112.3 (3)	H30B—C30—H30C	109.5
N2—C10—H10	110.7	C36—C31—C32	120.1 (3)
C19—C10—H10	110.7	C36—C31—N8	120.0 (3)
C11—C10—H10	110.7	C32—C31—N8	119.8 (3)
C12—C11—C10	102.8 (3)	C33—C32—C31	119.0 (3)
C12—C11—H11A	111.2	C33—C32—H32	120.5
C10—C11—H11A	111.2	C31—C32—H32	120.5
C12—C11—H11B	111.2	C32—C33—C34	121.9 (3)
C10—C11—H11B	111.2	C32—C33—H33	119.1
H11A—C11—H11B	109.1	C34—C33—H33	119.1
N3—C12—C13	121.8 (3)	C35—C34—C33	117.4 (3)
N3—C12—C11	114.1 (3)	C35—C34—C37	121.3 (3)
C13—C12—C11	124.1 (3)	C33—C34—C37	121.2 (3)
C14—C13—C18	118.4 (3)	C34—C35—C36	121.9 (3)
C14—C13—C12	120.8 (3)	C34—C35—H35	119.0
C18—C13—C12	120.8 (3)	C36—C35—H35	119.0
C15—C14—C13	121.3 (3)	C31—C36—C35	119.6 (3)
C15—C14—H14	119.4	C31—C36—H36	120.2
C13—C14—H14	119.4	C35—C36—H36	120.2
C16—C15—C14	118.6 (3)	C34—C37—H37A	109.5
C16—C15—H15	120.7	C34—C37—H37B	109.5
C14—C15—H15	120.7	H37A—C37—H37B	109.5

C15—C16—C17	121.5 (3)	C34—C37—H37C	109.5
C15—C16—Br2	119.1 (3)	H37A—C37—H37C	109.5
C17—C16—Br2	119.4 (3)	H37B—C37—H37C	109.5
C18—C17—C16	119.6 (4)	C9—N1—C7	109.3 (3)
C18—C17—H17	120.2	C9—N2—N3	119.7 (3)
C16—C17—H17	120.2	C9—N2—C10	125.2 (3)
C17—C18—C13	120.7 (4)	N3—N2—C10	113.9 (3)
C17—C18—H18	119.7	C12—N3—N2	108.3 (3)
C13—C18—H18	119.7	C20—N4—N5	112.1 (2)
C20—C19—C21	104.7 (3)	C20—N4—C22	127.2 (3)
C20—C19—C10	127.6 (3)	N5—N4—C22	120.6 (3)
C21—C19—C10	127.6 (3)	C21—N5—N4	104.1 (2)
N4—C20—C19	107.5 (3)	N7—N6—C28	109.2 (3)
N4—C20—H20	126.3	N6—N7—N8	107.1 (3)
C19—C20—H20	126.3	N7—N8—C29	111.3 (3)
N5—C21—C19	111.5 (3)	N7—N8—C31	119.3 (3)
N5—C21—C28	120.9 (3)	C29—N8—C31	129.4 (3)
C19—C21—C28	127.5 (3)	C8—S1—C9	87.66 (16)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···Br1^{i}	0.93	2.87	3.741 (3)	157

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