IUCrData

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3-[(3,5-Dimethyl-1*H*-pyrazol-1-yl)methyl]-4-(4-methylphenyl)-4,5-dihydro-1*H*-1,2,4-triazole-5-thione

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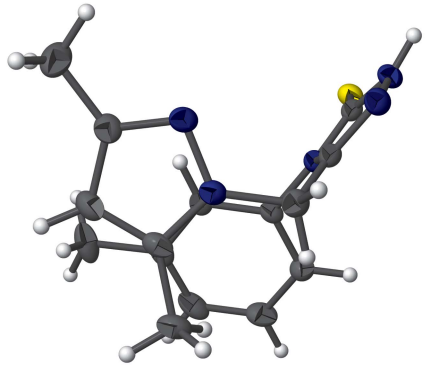
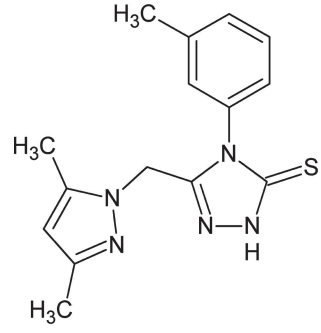
Structural data: full structural data are available from iucrdata.iucr.org

With the pyrazolyl and *p*-tolyl groups lying to one side of the plane through the linking 1,2,4-triazole-5-thione residue [forming dihedral angles of 87.05 (8) and 81.41 (7)°, respectively], the title molecule, $C_{15}H_{17}N_5S$, adopts a 'pincer' conformation stabilized in part by two intramolecular C—H···π(ring) interactions. A three-dimensional network structure is generated by a combination of intermolecular N—H···N and C—H···S hydrogen bonds, as well as C—H···π(ring) interactions.

3D view



Chemical scheme



Structure description

Pyrazoles and their derivatives are an important class of heterocyclic compounds due to their broad spectrum of biological properties. They exhibit anti-bacterial, anti-depressant (Liu *et al.*, 2008; Yhya *et al.*, 2012), anti-oxidant (Abdel-Aziz *et al.* 2009), anti-cancer (Grosse *et al.*, 2014) and anti-viral activities (Hamdy & El-Senousy, 2013) in addition to their anti-inflammatory and anti-microbial activities. Moreover, pyrazoles containing 4-substituted-1,2,4-triazole-3-thiones have been reported to possess anti-inflammatory activities (El-Moghazy *et al.*, 2012). As part of our research in this area, we report herein the synthesis and crystal structure of the title compound.

The title molecule adopts a 'pincer' conformation which is at least partly determined by two intramolecular C—H···π(ring) interactions (Table 1 and Fig. 1). The dihedral

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

*Cg*1, *Cg*2 and *Cg*3 are the centroids of the N1–N3/C1/C2, N4/N5/C11–C13 and C3–C8 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···*Cg*2	0.95	2.81	3.2544 (14)	110
C14—H14*A*···*Cg*3	0.98	2.79	3.6130 (17)	143
N3—H3*N*···N5^{i}	0.878 (18)	1.978 (18)	2.8334 (17)	164.5 (16)
C15—H15*C*···N2^{ii}	0.98	2.59	3.550 (2)	168
C9—H9*B*···*Cg*1^{ii}	0.98	2.88	3.637 (2)	135
C5—H5···S1^{iii}	0.95	2.93	3.824 (2)	157
C10—H10*A*···S1^{iv}	0.99	2.93	3.747 (1)	140

Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $x-1, y, z$; (iii) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (iv) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$.

angle between the C3–C8 and N1–N3/C1/C2 rings is 81.41 (7)° while that between the latter ring and the N4/N5,C11–C13 ring is 87.05 (8)°. Pairwise N3—H3···N5^{v} hydrogen bonds (Table 1) form dimers which are linked into a three-dimensional network by a combination of three sets of C—H···S hydrogen bonds and a set of C—H···π(ring) interactions (Table 1 and Figs. 2 and 3).

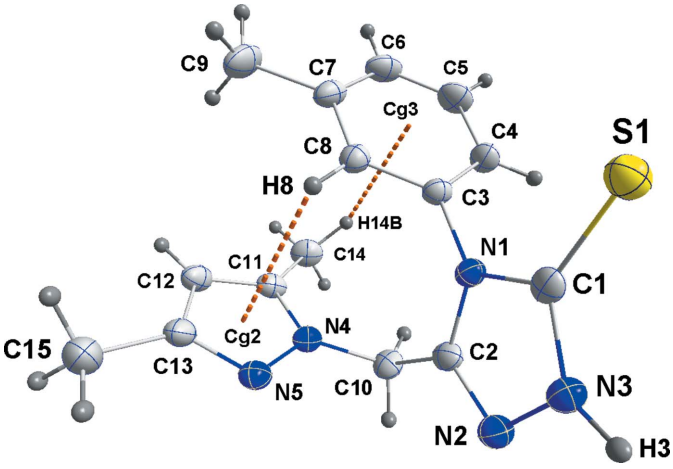


Figure 1
The title molecule with labelling scheme and 50% probability ellipsoids. The intramolecular C—H···π(ring) interactions are shown as dotted lines.

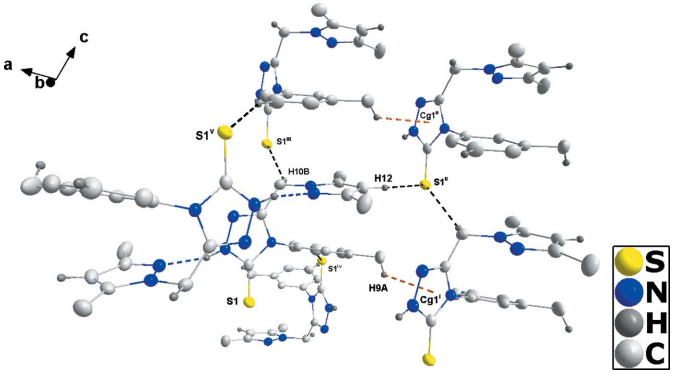


Figure 2
Detail of the intermolecular N—H···N (blue dotted lines) and C—H···S (black dotted lines) hydrogen bonds and the intermolecular C—H···π(ring) (orange dotted lines) interactions. [Symmetry codes: (i) $-1+x, y, z$; (ii) $-\frac{1}{2}+x, \frac{1}{2}-y, \frac{1}{2}+z$; (iii) $\frac{1}{2}+x, \frac{1}{2}-y, \frac{1}{2}+z$; (iv) $\frac{3}{2}-x, -\frac{1}{2}+y, \frac{1}{2}-z$.]

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_{17}N_5S$
M_r	299.39
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	150
a, b, c (Å)	7.9322 (2), 15.2415 (4), 13.6694 (4)
β (°)	106.316 (1)
V (Å^3)	1586.06 (7)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	1.81
Crystal size (mm)	0.15 × 0.15 × 0.07
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.82, 0.89
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11791, 3070, 2812
R_{int}	0.028
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.618
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.033, 0.091, 1.05
No. of reflections	3070
No. of parameters	191
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.24, −0.21

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

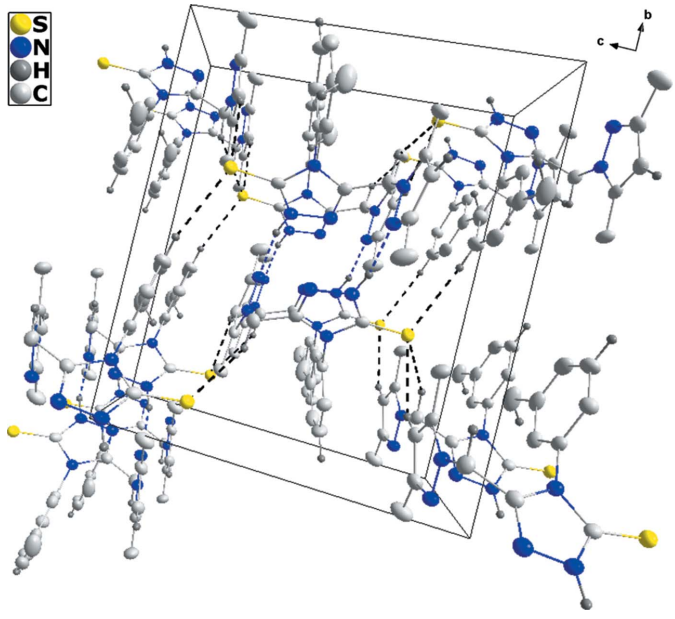


Figure 3
Packing viewed along the *a* axis. Intermolecular N—H···N and C—H···S hydrogen bonds are shown, respectively, as blue and black dotted lines.

Synthesis and crystallization

A solution of 2-(2-(3,5-dimethyl-1*H*-pyrazol-1-yl)acetyl)-*N*-*p*-tolylhydrazinecarbothioamide (1.27 g; 4 mmol) in ethanol (50 ml) was added dropwise to 2 *N* sodium hydroxide solution (20 ml). The reaction mixture was then refluxed for 2 h, cooled, filtered and the filtrate was acidified with 2 *N* hydrochloric acid solution. The separated solid was collected, washed with water and crystallized from ethanol solution.

Refinement

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

Acknowledgements

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full crystallographic data

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Crystal data

$C_{15}H_{17}N_5S$
M_r = 299.39
Monoclinic, $P2_1/n$
a = 7.9322 (2) Å
b = 15.2415 (4) Å
c = 13.6694 (4) Å
β = 106.316 (1)°
V = 1586.06 (7) Å^3
Z = 4
$F(000)$ = 632
D_x = 1.254 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9878 reflections
θ = 2.9–72.4°
μ = 1.81 mm^{-1}
T = 150 K
Thick plate, colourless
0.15 × 0.15 × 0.07 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} = 0.82, T_{max} = 0.89
11791 measured reflections
3070 independent reflections
2812 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 72.4°, θ_{min} = 4.5°
h = −9→9
k = −18→18
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.091
S = 1.05
3070 reflections
191 parameters
0 restraints
Hydrogen site location: mixed
$w = 1/[\sigma^2(F_o^2) + (0.0454P)^2 + 0.6677P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Extinction correction: SHELXL2014 (Sheldrick, 2015*b*), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0040 (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	0.92398 (17)	0.37412 (8)	0.35362 (10)	0.0212 (2)
C2	1.00943 (17)	0.35248 (9)	0.52192 (10)	0.0212 (2)
C3	0.77405 (17)	0.25167 (9)	0.41923 (9)	0.0204 (3)
C4	0.82341 (19)	0.16998 (9)	0.39224 (11)	0.0268 (3)
H4	0.9348	0.1617	0.3805	0.032*
C5	0.7066 (2)	0.10048 (10)	0.38268 (12)	0.0341 (4)
H5	0.7370	0.0442	0.3631	0.041*
C6	0.5455 (2)	0.11329 (11)	0.40169 (11)	0.0341 (4)
H6	0.4673	0.0651	0.3957	0.041*
C7	0.49608 (19)	0.19490 (11)	0.42931 (10)	0.0290 (3)
C8	0.61277 (17)	0.26505 (9)	0.43697 (10)	0.0230 (3)
H8	0.5812	0.3219	0.4544	0.028*
C9	0.3242 (2)	0.20843 (14)	0.45340 (13)	0.0435 (4)
H9A	0.2501	0.1564	0.4327	0.065*
H9B	0.2644	0.2598	0.4163	0.065*
H9C	0.3461	0.2178	0.5268	0.065*
C10	1.01710 (18)	0.31858 (10)	0.62551 (10)	0.0257 (3)
H10A	1.0425	0.2549	0.6284	0.031*
H10B	1.1139	0.3481	0.6768	0.031*
C11	0.74452 (19)	0.27428 (9)	0.67525 (10)	0.0245 (3)
C12	0.6022 (2)	0.32088 (10)	0.68573 (11)	0.0273 (3)
H12	0.5029	0.2982	0.7032	0.033*
C13	0.63305 (19)	0.40877 (9)	0.66543 (11)	0.0263 (3)
C14	0.7851 (2)	0.17859 (10)	0.68567 (12)	0.0327 (3)
H14A	0.7884	0.1549	0.6196	0.049*
H14B	0.6940	0.1482	0.7086	0.049*
H14C	0.8995	0.1698	0.7357	0.049*
C15	0.5202 (2)	0.48732 (11)	0.66467 (15)	0.0405 (4)
H15A	0.5736	0.5388	0.6424	0.061*
H15B	0.5095	0.4975	0.7335	0.061*
H15C	0.4034	0.4772	0.6177	0.061*
N1	0.89554 (14)	0.32359 (7)	0.43150 (8)	0.0202 (2)
N2	1.10763 (15)	0.41591 (8)	0.50617 (9)	0.0250 (3)
N3	1.05596 (15)	0.42747 (8)	0.40224 (9)	0.0238 (3)
H3N	1.093 (2)	0.4738 (12)	0.3762 (13)	0.029*
N4	0.85295 (15)	0.33364 (7)	0.65030 (8)	0.0223 (2)
N5	0.78636 (15)	0.41691 (7)	0.64379 (9)	0.0242 (3)
S1	0.81896 (4)	0.36931 (2)	0.22924 (2)	0.02550 (13)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0196 (4)	0.0185 (5)	0.0261 (5)	0.0009 (3)	0.0076 (4)	−0.0015 (3)
C2	0.0196 (4)	0.0185 (5)	0.0261 (5)	0.0009 (3)	0.0076 (4)	−0.0015 (3)
C3	0.0216 (6)	0.0199 (6)	0.0190 (6)	−0.0040 (5)	0.0045 (5)	0.0010 (5)
C4	0.0271 (7)	0.0236 (7)	0.0307 (7)	−0.0008 (5)	0.0099 (6)	−0.0023 (6)
C5	0.0444 (9)	0.0219 (7)	0.0356 (8)	−0.0068 (6)	0.0106 (7)	−0.0046 (6)
C6	0.0377 (8)	0.0338 (8)	0.0283 (7)	−0.0171 (7)	0.0052 (6)	0.0003 (6)
C7	0.0227 (7)	0.0417 (9)	0.0206 (6)	−0.0085 (6)	0.0031 (5)	0.0032 (6)
C8	0.0209 (6)	0.0272 (7)	0.0200 (6)	−0.0003 (5)	0.0042 (5)	0.0013 (5)
C9	0.0254 (8)	0.0717 (13)	0.0345 (8)	−0.0139 (8)	0.0098 (6)	−0.0007 (8)
C10	0.0222 (7)	0.0287 (7)	0.0245 (7)	0.0012 (5)	0.0037 (5)	0.0025 (5)
C11	0.0310 (7)	0.0229 (7)	0.0181 (6)	−0.0058 (5)	0.0046 (5)	0.0018 (5)
C12	0.0311 (7)	0.0281 (8)	0.0249 (7)	−0.0085 (6)	0.0114 (6)	−0.0027 (6)
C13	0.0263 (7)	0.0256 (7)	0.0270 (7)	−0.0052 (5)	0.0077 (6)	−0.0060 (6)
C14	0.0397 (9)	0.0235 (8)	0.0328 (8)	−0.0026 (6)	0.0069 (7)	0.0069 (6)
C15	0.0316 (8)	0.0315 (9)	0.0593 (11)	−0.0026 (6)	0.0141 (8)	−0.0134 (8)
N1	0.0187 (5)	0.0188 (6)	0.0232 (5)	−0.0019 (4)	0.0062 (4)	−0.0005 (4)
N2	0.0227 (6)	0.0247 (6)	0.0273 (6)	−0.0029 (4)	0.0062 (5)	−0.0020 (5)
N3	0.0254 (6)	0.0202 (6)	0.0272 (6)	−0.0047 (4)	0.0094 (5)	−0.0004 (5)
N4	0.0237 (6)	0.0209 (6)	0.0213 (5)	−0.0012 (4)	0.0047 (4)	0.0018 (4)
N5	0.0253 (6)	0.0198 (6)	0.0267 (6)	−0.0026 (4)	0.0059 (5)	−0.0008 (4)
S1	0.0306 (2)	0.0232 (2)	0.02287 (19)	−0.00195 (12)	0.00779 (14)	0.00007 (12)

Geometric parameters (Å, º)

C1—N3	1.3446 (17)	C9—H9C	0.9800
C1—N1	1.3830 (17)	C10—N4	1.4528 (18)
C1—S1	1.6716 (14)	C10—H10A	0.9900
C2—N2	1.2969 (18)	C10—H10B	0.9900
C2—N1	1.3821 (17)	C11—N4	1.3562 (17)
C2—C10	1.4925 (18)	C11—C12	1.375 (2)
C3—C8	1.3825 (19)	C11—C14	1.492 (2)
C3—C4	1.3860 (19)	C12—C13	1.403 (2)
C3—N1	1.4378 (16)	C12—H12	0.9500
C4—C5	1.389 (2)	C13—N5	1.3356 (19)
C4—H4	0.9500	C13—C15	1.493 (2)
C5—C6	1.387 (2)	C14—H14A	0.9800
C5—H5	0.9500	C14—H14B	0.9800
C6—C7	1.388 (2)	C14—H14C	0.9800
C6—H6	0.9500	C15—H15A	0.9800
C7—C8	1.399 (2)	C15—H15B	0.9800
C7—C9	1.504 (2)	C15—H15C	0.9800
C8—H8	0.9500	N2—N3	1.3749 (16)
C9—H9A	0.9800	N3—H3N	0.877 (18)
C9—H9B	0.9800	N4—N5	1.3680 (16)

N3—C1—N1	103.24 (11)	C2—C10—H10B	109.3
N3—C1—S1	128.72 (11)	H10A—C10—H10B	108.0
N1—C1—S1	128.04 (10)	N4—C11—C12	106.20 (12)
N2—C2—N1	111.18 (12)	N4—C11—C14	122.77 (13)
N2—C2—C10	123.31 (12)	C12—C11—C14	131.03 (13)
N1—C2—C10	125.47 (12)	C11—C12—C13	106.16 (12)
C8—C3—C4	121.58 (13)	C11—C12—H12	126.9
C8—C3—N1	119.34 (12)	C13—C12—H12	126.9
C4—C3—N1	119.06 (12)	N5—C13—C12	110.66 (13)
C3—C4—C5	118.64 (14)	N5—C13—C15	120.36 (13)
C3—C4—H4	120.7	C12—C13—C15	128.98 (14)
C5—C4—H4	120.7	C11—C14—H14A	109.5
C6—C5—C4	120.01 (15)	C11—C14—H14B	109.5
C6—C5—H5	120.0	H14A—C14—H14B	109.5
C4—C5—H5	120.0	C11—C14—H14C	109.5
C5—C6—C7	121.50 (14)	H14A—C14—H14C	109.5
C5—C6—H6	119.3	H14B—C14—H14C	109.5
C7—C6—H6	119.3	C13—C15—H15A	109.5
C6—C7—C8	118.28 (13)	C13—C15—H15B	109.5
C6—C7—C9	121.68 (14)	H15A—C15—H15B	109.5
C8—C7—C9	120.03 (15)	C13—C15—H15C	109.5
C3—C8—C7	119.98 (13)	H15A—C15—H15C	109.5
C3—C8—H8	120.0	H15B—C15—H15C	109.5
C7—C8—H8	120.0	C2—N1—C1	107.70 (11)
C7—C9—H9A	109.5	C2—N1—C3	126.55 (11)
C7—C9—H9B	109.5	C1—N1—C3	125.71 (11)
H9A—C9—H9B	109.5	C2—N2—N3	104.38 (11)
C7—C9—H9C	109.5	C1—N3—N2	113.45 (11)
H9A—C9—H9C	109.5	C1—N3—H3N	126.1 (11)
H9B—C9—H9C	109.5	N2—N3—H3N	119.0 (11)
N4—C10—C2	111.49 (11)	C11—N4—N5	112.00 (11)
N4—C10—H10A	109.3	C11—N4—C10	128.80 (12)
C2—C10—H10A	109.3	N5—N4—C10	119.10 (11)
N4—C10—H10B	109.3	C13—N5—N4	104.98 (11)

C8—C3—C4—C5	0.2 (2)	N3—C1—N1—C3	−175.76 (12)
N1—C3—C4—C5	178.65 (12)	S1—C1—N1—C3	4.15 (19)
C3—C4—C5—C6	−1.1 (2)	C8—C3—N1—C2	82.53 (16)
C4—C5—C6—C7	0.7 (2)	C4—C3—N1—C2	−95.92 (16)
C5—C6—C7—C8	0.5 (2)	C8—C3—N1—C1	−100.26 (15)
C5—C6—C7—C9	−177.92 (14)	C4—C3—N1—C1	81.29 (16)
C4—C3—C8—C7	1.0 (2)	N1—C2—N2—N3	−0.52 (15)
N1—C3—C8—C7	−177.44 (11)	C10—C2—N2—N3	−178.55 (12)
C6—C7—C8—C3	−1.3 (2)	N1—C1—N3—N2	−2.35 (15)
C9—C7—C8—C3	177.12 (13)	S1—C1—N3—N2	177.75 (10)
N2—C2—C10—N4	115.87 (14)	C2—N2—N3—C1	1.86 (15)
N1—C2—C10—N4	−61.87 (17)	C12—C11—N4—N5	−0.22 (15)
N4—C11—C12—C13	0.25 (15)	C14—C11—N4—N5	179.05 (12)

C14—C11—C12—C13	−178.93 (14)	C12—C11—N4—C10	−176.50 (12)
C11—C12—C13—N5	−0.21 (16)	C14—C11—N4—C10	2.8 (2)
C11—C12—C13—C15	179.17 (15)	C2—C10—N4—C11	121.63 (14)
N2—C2—N1—C1	−0.89 (15)	C2—C10—N4—N5	−54.42 (16)
C10—C2—N1—C1	177.09 (12)	C12—C13—N5—N4	0.08 (15)
N2—C2—N1—C3	176.74 (12)	C15—C13—N5—N4	−179.37 (13)
C10—C2—N1—C3	−5.3 (2)	C11—N4—N5—C13	0.09 (14)
N3—C1—N1—C2	1.89 (14)	C10—N4—N5—C13	176.77 (11)
S1—C1—N1—C2	−178.20 (10)		

Hydrogen-bond geometry (Å, º)

Cg1, Cg2 and Cg3 are the centroids of the N1–N3/C1/C2, N4/N5/C11–C13 and C3–C8 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···*Cg*2	0.95	2.81	3.2544 (14)	110
C14—H14*A*···*Cg*3	0.98	2.79	3.6130 (17)	143
N3—H3*N*···N5^{i}	0.878 (18)	1.978 (18)	2.8334 (17)	164.5 (16)
C15—H15*C*···N2^{ii}	0.98	2.59	3.550 (2)	168
C9—H9*B*···*Cg*1^{ii}	0.98	2.88	3.637 (2)	135
C5—H5···S1^{iii}	0.95	2.93	3.824 (2)	157
C10—H10*A*···S1^{iv}	0.99	2.93	3.747 (1)	140

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