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Crystal structure of 2-[(3a*S*,6*R*)-3,3,6-trimethyl-3,3a,4,5,6,7-hexahydro-2*H*-indazol-2-yl]thiazol-4(5*H*)-one

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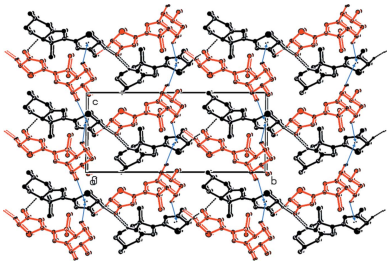
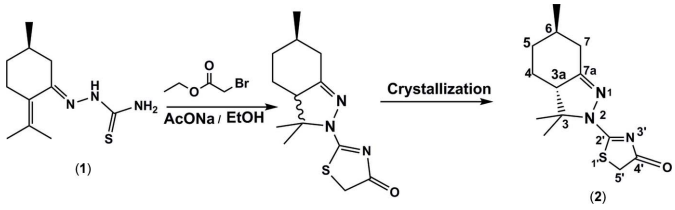
The title compound, $C_{13}H_{19}N_3OS$, is a new thiazolidin-4-one derivative prepared and isolated as the pure (3a*S*,6*R*)-diastereisomer from (*R*)-thiosemicarbazone pulegone. It crystallized with two independent molecules (*A* and *B*) in the asymmetric unit. The compound is composed of a hexhydroindazole ring system (*viz.* a five-membered dihydropyrazole ring fused to a cyclohexyl ring) with a thiazole-4-one ring system attached to one of the pyrazole N atoms (at position 2). The overall geometry of the two molecules differs slightly, with the mean planes of the pyrazole and thiazole rings being inclined to one another by 10.4 (1)° in molecule *A* and 0.9 (1)° in molecule *B*. In the crystal, the *A* and *B* molecules are linked *via* C—H···O hydrogen bonds, forming slabs parallel to the *ab* plane. There are C—H···π interactions present within the layers, and between the layers, so forming a three-dimensional structure.

1. Chemical context

Thiazolidinones constitute an important class of heterocyclic compounds containing sulfur and nitrogen in a five-membered ring. They play a vital role due to their wide range of biological activities and industrial importance. Thiazolidin-4-ones are particularly important because of their efficiency towards various pharmacological usages. A recent literature search reveals that thiazolidin-4-one derivatives may exhibit antibacterial (Bonde & Gaikwad, 2004), antituberculosis (Karali *et al.*, 2007), antiviral (Kaushik-Basu *et al.*, 2008) and anticancer activities (Patel *et al.*, 2014).

As a part of our endeavour toward the preparation of new heterocyclic systems, we report herein on the structure of a new optically active thiazolidin-4-one (**2**) synthesized from (*R*)-thiosemicarbazone pulegone (**1**); see Scheme. The reaction involves the treatment of thiosemicarbazone (**1**), in





refluxing ethanol, with ethyl bromoacatete and an excess of sodium acetate. Crystallization from an ethanolic solution of the resulting indazolic thiazolidin-4-one (obtained as a

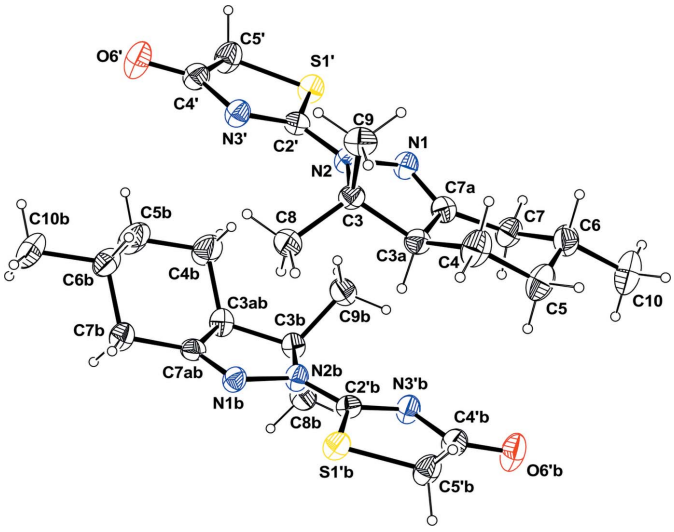


Figure 1
View of the molecular structure of the two independent molecules (*A* and *B*) of the title compound, showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

diastereomeric mixture) led to the isolation of compound (**2**). The structure of (**2**) was elucidated using spectroscopic (MS and NMR) data, while its absolute structure was determined as (3a*S*,6*R*) based mainly on the synthetic pathway and confirmed by resonant scattering.

2. Structural commentary

The title compound crystallized with two independent molecules (*A* and *B*) in the asymmetric unit. The compound is composed of a hexhydroindazole ring system [*viz.* a five-membered dihydropyrazole ring fused to a cyclohexyl ring] with a thiazole-4-one ring system attached to pyrazole N atom N2 (Fig. 1). Molecular fitting of the two molecules (Spek, 2009) shows that they have roughly the same conformation and the same configuration (Fig. 2), even if some slight differences can be observed. The six-membered rings each display a chair conformation, with puckering parameters of θ = 12.96° and φ2 = 113.49° for molecule *A* and θ = 9.44° and φ2 = 92.43° for molecule *B*. The five-membered pyrazol rings are almost planar with the largest deviation being 0.081 (3) Å for atom C3 in molecule *A* and −0.032 (1) for atom C3*B* in molecule *B*. The thiazole rings are planar, the largest deviation being −0.011 (1) Å for atom C2′ and 0.005 (1) for atom C5′*B* in molecules *A* and *B*, respectively. In molecule *A*, the two five-membered rings are slightly twisted with a dihedral angle of 10.4 (1)°, whereas in molecule *B* the two rings are almost coplanar with a dihedral angle of 0.9 (1)°.

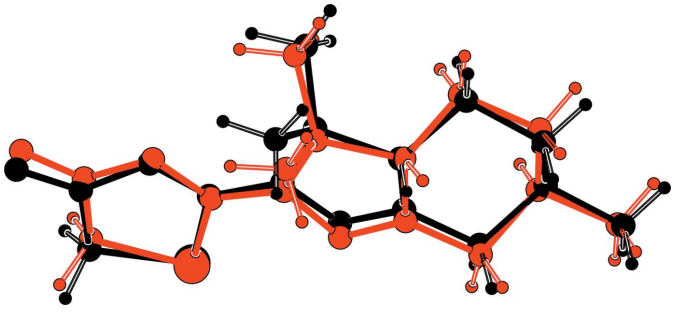


Figure 2
Molecular fitting of independent molecules *A* (black) and *B* (red).

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

*Cg*1 is the centroid of the thiazole ring S1′/N3′/C2′/C4′/C5′.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5′—H5′2···O6′*B*^{i}	0.97	2.43	3.304 (4)	150
C9—H9*B*···O6′*B*^{ii}	0.96	2.53	3.361 (3)	145
C5′*B*—H5′3···O6′^{iii}	0.97	2.44	3.361 (3)	159
C4*B*—H4*B*2···*Cg*1	0.96	2.93	3.737 (4)	141
C7*B*—H7*B*2···*Cg*1^{iv}	0.96	2.90	3.867 (4)	174

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

3. Supramolecular features

In the crystal, the two independent molecules are connected *via* C—H···O hydrogen bonds forming layers, or slabs, parallel to the *ab* plane (Table 1 and Fig. 3). Within the layers there are C—H···π interactions present (Fig. 4 and Table 1). The layers are also linked by C—H···π interactions (Table 1), forming a three-dimensional structure (Fig. 4).

4. Database survey

A search of the Cambridge Structural Database (CSD, V5.37, update November 2015; Groom & Allen, 2014) using the hexahydroindazole ring system as the main skeleton, revealed the presence of 27 structures. A search for a thiazole ring

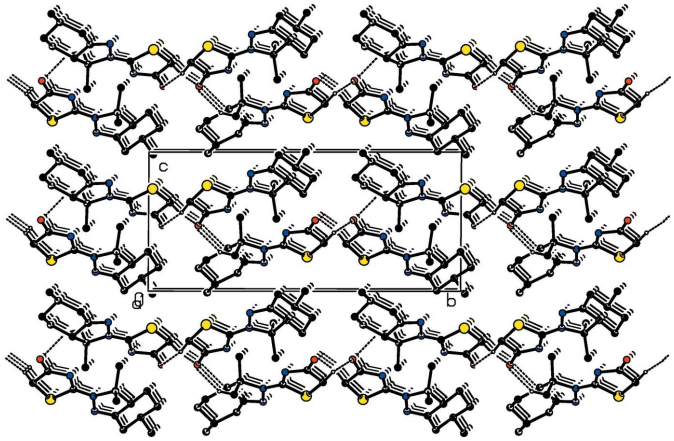


Figure 3
A view along the *a* axis of the crystal packing of the title compound, showing the formation of layers parallel to the *ab* plane *via* C—H···O hydrogen bonds (see Table 1). H atoms not involved in these interactions have been omitted for clarity.

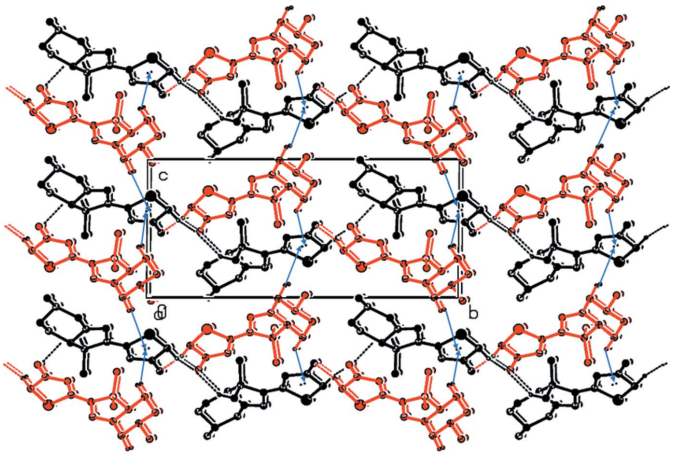


Figure 4
A view along the *a* axis of the crystal packing of the title compound, showing the C—H···O hydrogen bonds (dashed lines), and the C—H···π interactions (represented by blue arrows) linking the *A* (black) and *B* (red) molecules within and between the layers (see Table 1). H atoms not involved in these interactions have been omitted for clarity.

linked to an N atom of a pyrazole ring, similar to the situation in the title compound, yielded six hits. One of these structures, 2-(3-phenyl-3,3a,4,5-tetrahydro-2*H*-benzo[*g*]indazol-2-yl)-1,3-thiazol-4(5*H*)-one (refcode LUHGAY; Gautam & Chaudhary, 2015), resembles the title compound with an indazole ring system linked to a thiazole ring. The mean plane of the two five-membered rings are inclined to one another by *ca* 10.05°, similar to the arrangement in molecule *A* of the title compound.

5. Synthesis and crystallization

The synthesis of the title compound is illustrated in the Scheme. A mixture of thiosemicarbazone (**1**) (1.5 mmol, 1 eq), ethyl 2-bromoacetate (0.24 ml, 1.5 mmol) and anhydrous sodium acetate (0.37 g, 4.5 mmol, 3 eq) in absolute ethanol (30 ml) was heated under reflux until the completion of the reaction (1–3 h). The solvent was then evaporated under reduced pressure and the crude product was purified by chromatography on silica gel (230–400 mesh) using hexane/ethyl acetate (90:10) as eluent to give pure indazolic thiazolidin-4-one in 60% yield as a diastereomeric mixture. Slow evaporation from an ethanolic solution gives crystals of the pure diastereoisomer of the title compound (**2**) suitable for crystallographic analysis.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The C-bound H atoms were included in calculated positions and treated as riding atoms: C—H = 0.96–0.98 Å with U_{iso}(H) = 1.5U_{eq}(C-methyl) and 1.2U_{eq}(C) for other H atoms.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{13}H_{19}N_3OS$
M_r	265.37
Crystal system, space group	Monoclinic, $P2_1$
Temperature (K)	180
a, *b*, *c* (Å)	8.5519 (2), 18.9335 (4), 8.9165 (3)
β (°)	110.203 (3)
V (Å^3)	1354.91 (7)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.23
Crystal size (mm)	0.25 × 0.21 × 0.18
Data collection	
Diffractometer	Agilent Xcalibur Eos Gemini ultra
Absorption correction	Multi-scan (*CrysAlis PRO*; Agilent, 2014)
T_{min}, T_{max}	0.939, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	15302, 6147, 5674
R_{int}	0.024
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.692
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.033, 0.077, 1.04
No. of reflections	6147
No. of parameters	331
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.22, −0.19
Absolute structure	Flack *x* determined using 2349 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	−0.08 (3)

Computer programs: *CrysAlis PRO* (Agilent, 2014), *SIR97* (Altomare *et al.*, 1999), *SHELXL2013* (Sheldrick, 2015), *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009).

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Crystal structure of 2-[(3a*S*,6*R*)-3,3,6-trimethyl-3,3a,4,5,6,7-hexahydro-2*H*-indazol-2-yl]thiazol-4(5*H*)-one

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Computing details

Data collection: *CrysAlis PRO* (Agilent, 2014); cell refinement: *CrysAlis PRO* (Agilent, 2014); data reduction: *CrysAlis PRO* (Agilent, 2014); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2015); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL2013* (Sheldrick, 2015).

2-[(3a*S*,6*R*)-3,3,6-Trimethyl-3,3a,4,5,6,7-hexahydro-2*H*-indazol-2-yl]thiazol-4(5*H*)-one

Crystal data

$C_{13}H_{19}N_3OS$
$M_r = 265.37$
Monoclinic, $P2_1$
$a = 8.5519$ (2) Å
$b = 18.9335$ (4) Å
$c = 8.9165$ (3) Å
$\beta = 110.203$ (3)°
$V = 1354.91$ (7) Å^3
$Z = 4$
$F(000) = 568$
$D_x = 1.301$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5859 reflections
$\theta = 3.6$–$29.2°$
$\mu = 0.23$ mm^{-1}
$T = 180$ K
Prismatic, colourless
0.25 × 0.21 × 0.18 mm

Data collection

Agilent Xcalibur Eos Gemini ultra diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 16.1978 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2014)
$T_{min} = 0.939$, $T_{max} = 1.000$
15302 measured reflections
6147 independent reflections
5674 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 29.5°$, $\theta_{min} = 3.3°$
$h = -11 \rightarrow 11$
$k = -23 \rightarrow 25$
$l = -12 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.077$
$S = 1.04$
6147 reflections
331 parameters
1 restraint
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0364P)^2 + 0.1555P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.22$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}

Absolute structure: Flack *x* determined using 2349 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: −0.08 (3)

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}
S1′	0.77265 (7)	0.51418 (3)	0.26117 (7)	0.02894 (15)
O6′	1.2287 (2)	0.54265 (10)	0.5307 (3)	0.0410 (5)
N1	0.6528 (2)	0.37534 (10)	0.2176 (2)	0.0258 (4)
N2	0.8216 (2)	0.37680 (10)	0.3163 (2)	0.0246 (4)
N3′	1.0511 (3)	0.44868 (11)	0.4370 (2)	0.0269 (4)
C2′	0.8954 (3)	0.43930 (12)	0.3469 (3)	0.0232 (5)
C4′	1.0915 (3)	0.51929 (14)	0.4524 (3)	0.0290 (5)
C5′	0.9500 (3)	0.56889 (15)	0.3626 (3)	0.0358 (6)
H5′1	0.9808	0.5970	0.2862	0.043*
H5′2	0.9245	0.6005	0.4366	0.043*
C3	0.8934 (3)	0.30406 (12)	0.3685 (3)	0.0241 (5)
C3A	0.7284 (3)	0.26108 (13)	0.3219 (3)	0.0266 (5)
H3A	0.7035	0.2524	0.4197	0.032*
C4	0.7166 (3)	0.19101 (16)	0.2363 (3)	0.0389 (6)
H4A	0.7865	0.1564	0.3091	0.047*
H4B	0.7564	0.1965	0.1474	0.047*
C5	0.5357 (4)	0.16515 (15)	0.1746 (4)	0.0406 (7)
H5A	0.5305	0.1200	0.1216	0.049*
H5B	0.4984	0.1580	0.2645	0.049*
C6	0.4191 (3)	0.21710 (15)	0.0582 (3)	0.0356 (6)
H6	0.4574	0.2231	−0.0327	0.043*
C7	0.4263 (3)	0.28925 (13)	0.1385 (3)	0.0318 (5)
H7A	0.3692	0.3240	0.0583	0.038*
H7B	0.3690	0.2864	0.2151	0.038*
C7A	0.6020 (3)	0.31236 (12)	0.2218 (3)	0.0257 (5)
C9	1.0058 (3)	0.28524 (14)	0.2749 (3)	0.0318 (5)
H9A	0.9442	0.2890	0.1625	0.048*
H9B	1.0454	0.2377	0.2997	0.048*
H9C	1.0988	0.3171	0.3031	0.048*
C8	0.9873 (3)	0.30082 (14)	0.5474 (3)	0.0331 (6)
H8A	1.0870	0.3286	0.5732	0.050*
H8B	1.0161	0.2527	0.5787	0.050*
H8C	0.9182	0.3191	0.6033	0.050*
C10	0.2398 (4)	0.1906 (2)	−0.0055 (4)	0.0551 (8)

H10A	0.2358	0.1458	−0.0573	0.083*
H10B	0.1715	0.2240	−0.0808	0.083*
H10C	0.1990	0.1852	0.0816	0.083*
S1′B	0.72290 (7)	0.19227 (3)	0.77175 (8)	0.02873 (15)
O6′B	0.2793 (2)	0.16136 (10)	0.4764 (3)	0.0430 (5)
N1B	0.8189 (2)	0.33287 (10)	0.8585 (2)	0.0256 (4)
N2B	0.6558 (2)	0.32950 (10)	0.7482 (2)	0.0251 (4)
N3′B	0.4417 (3)	0.25589 (11)	0.5972 (2)	0.0285 (4)
C2′B	0.5933 (3)	0.26630 (13)	0.6977 (3)	0.0231 (5)
C4′B	0.4099 (3)	0.18550 (14)	0.5654 (3)	0.0297 (5)
C5′B	0.5556 (3)	0.13661 (14)	0.6521 (3)	0.0323 (6)
H5′3	0.5899	0.1101	0.5756	0.039*
H5′4	0.5236	0.1035	0.7194	0.039*
C3B	0.5720 (3)	0.40092 (12)	0.7089 (3)	0.0243 (5)
C3AB	0.7198 (3)	0.44937 (13)	0.8040 (3)	0.0272 (5)
H3AB	0.6873	0.4763	0.8825	0.033*
C4B	0.7936 (4)	0.50042 (17)	0.7135 (4)	0.0458 (7)
H4B1	0.7139	0.5375	0.6651	0.055*
H4B2	0.8175	0.4754	0.6290	0.055*
C5B	0.9540 (4)	0.53296 (16)	0.8284 (4)	0.0483 (8)
H5B1	0.9978	0.5662	0.7701	0.058*
H5B2	0.9282	0.5590	0.9106	0.058*
C6B	1.0865 (3)	0.47829 (14)	0.9071 (3)	0.0334 (6)
H6B	1.1154	0.4540	0.8231	0.040*
C7B	1.0200 (3)	0.42344 (13)	0.9955 (3)	0.0309 (5)
H7B1	1.0964	0.3838	1.0262	0.037*
H7B2	1.0117	0.4442	1.0919	0.037*
C7AB	0.8528 (3)	0.39813 (13)	0.8913 (3)	0.0250 (5)
C9B	0.5074 (3)	0.41293 (14)	0.5291 (3)	0.0328 (6)
H9B1	0.4216	0.3791	0.4788	0.049*
H9B2	0.5971	0.4075	0.4886	0.049*
H9B3	0.4625	0.4598	0.5064	0.049*
C8B	0.4338 (3)	0.40513 (15)	0.7789 (3)	0.0321 (6)
H8B1	0.3807	0.4505	0.7553	0.048*
H8B2	0.4799	0.3988	0.8926	0.048*
H8B3	0.3533	0.3687	0.7330	0.048*
C10B	1.2448 (3)	0.51173 (18)	1.0226 (4)	0.0468 (7)
H10D	1.2862	0.5463	0.9669	0.070*
H10E	1.3276	0.4758	1.0650	0.070*
H10F	1.2202	0.5341	1.1085	0.070*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1′	0.0251 (3)	0.0232 (3)	0.0350 (3)	0.0039 (3)	0.0059 (3)	0.0028 (2)
O6′	0.0283 (10)	0.0288 (10)	0.0563 (12)	−0.0043 (8)	0.0025 (10)	−0.0012 (9)
N1	0.0204 (10)	0.0254 (10)	0.0294 (11)	0.0025 (8)	0.0058 (8)	−0.0001 (8)
N2	0.0189 (10)	0.0229 (10)	0.0299 (10)	0.0017 (8)	0.0059 (8)	0.0029 (8)

N3′	0.0226 (10)	0.0242 (10)	0.0311 (11)	0.0008 (8)	0.0057 (9)	0.0023 (8)
C2′	0.0254 (12)	0.0218 (12)	0.0237 (11)	0.0035 (9)	0.0103 (10)	0.0022 (9)
C4′	0.0276 (13)	0.0272 (13)	0.0320 (12)	−0.0002 (11)	0.0100 (11)	0.0012 (11)
C5′	0.0315 (14)	0.0259 (14)	0.0447 (15)	−0.0006 (12)	0.0065 (13)	0.0030 (11)
C3	0.0236 (11)	0.0207 (11)	0.0265 (12)	0.0019 (9)	0.0068 (10)	0.0049 (9)
C3A	0.0271 (12)	0.0266 (12)	0.0260 (11)	−0.0003 (10)	0.0089 (10)	0.0019 (10)
C4	0.0365 (15)	0.0238 (13)	0.0521 (17)	0.0023 (12)	0.0098 (13)	−0.0040 (13)
C5	0.0401 (16)	0.0269 (14)	0.0529 (17)	−0.0061 (12)	0.0138 (14)	−0.0103 (13)
C6	0.0362 (15)	0.0388 (14)	0.0319 (13)	−0.0079 (12)	0.0121 (12)	−0.0107 (12)
C7	0.0255 (12)	0.0298 (13)	0.0381 (14)	−0.0006 (10)	0.0083 (11)	−0.0009 (11)
C7A	0.0262 (12)	0.0255 (12)	0.0261 (12)	0.0021 (9)	0.0099 (10)	−0.0025 (9)
C9	0.0302 (13)	0.0313 (13)	0.0353 (13)	0.0074 (11)	0.0130 (11)	0.0061 (11)
C8	0.0343 (14)	0.0337 (14)	0.0273 (13)	−0.0018 (11)	0.0055 (11)	0.0051 (10)
C10	0.0411 (17)	0.0507 (19)	0.064 (2)	−0.0136 (17)	0.0065 (16)	−0.0210 (17)
S1′B	0.0231 (3)	0.0223 (3)	0.0364 (3)	0.0027 (2)	0.0046 (3)	0.0057 (2)
O6′B	0.0303 (11)	0.0298 (10)	0.0540 (12)	−0.0032 (9)	−0.0044 (10)	−0.0025 (9)
N1B	0.0193 (9)	0.0254 (11)	0.0285 (10)	−0.0003 (8)	0.0037 (8)	0.0039 (8)
N2B	0.0201 (10)	0.0224 (10)	0.0283 (10)	0.0031 (8)	0.0025 (8)	0.0012 (8)
N3′B	0.0249 (11)	0.0225 (10)	0.0324 (11)	0.0010 (9)	0.0025 (9)	0.0008 (9)
C2′B	0.0215 (12)	0.0232 (12)	0.0254 (11)	0.0024 (9)	0.0089 (10)	0.0034 (9)
C4′B	0.0268 (13)	0.0262 (13)	0.0335 (13)	−0.0005 (11)	0.0072 (11)	0.0009 (11)
C5′B	0.0287 (14)	0.0204 (13)	0.0422 (15)	0.0004 (11)	0.0054 (12)	0.0033 (11)
C3B	0.0243 (12)	0.0206 (11)	0.0256 (12)	0.0048 (9)	0.0056 (10)	0.0000 (9)
C3AB	0.0257 (12)	0.0250 (12)	0.0306 (13)	0.0032 (9)	0.0093 (10)	−0.0053 (10)
C4B	0.0447 (17)	0.0318 (16)	0.0514 (18)	−0.0054 (12)	0.0043 (14)	0.0139 (13)
C5B	0.0503 (18)	0.0270 (15)	0.062 (2)	−0.0110 (13)	0.0127 (16)	0.0076 (13)
C6B	0.0315 (14)	0.0320 (14)	0.0414 (15)	−0.0078 (11)	0.0187 (12)	−0.0081 (11)
C7B	0.0247 (12)	0.0320 (13)	0.0341 (13)	−0.0027 (10)	0.0077 (10)	−0.0014 (11)
C7AB	0.0260 (12)	0.0281 (12)	0.0230 (11)	−0.0009 (10)	0.0111 (10)	0.0021 (9)
C9B	0.0398 (14)	0.0280 (13)	0.0285 (13)	0.0026 (11)	0.0090 (12)	0.0000 (10)
C8B	0.0262 (12)	0.0385 (14)	0.0315 (13)	0.0035 (11)	0.0100 (11)	−0.0004 (11)
C10B	0.0370 (16)	0.0417 (17)	0.0629 (19)	−0.0179 (15)	0.0190 (15)	−0.0129 (16)

Geometric parameters (Å, º)

S1′—C2′	1.772 (2)	S1′B—C2′B	1.767 (2)
S1′—C5′	1.801 (3)	S1′B—C5′B	1.800 (3)
O6′—C4′	1.222 (3)	O6′B—C4′B	1.214 (3)
N1—C7A	1.274 (3)	N1B—C7AB	1.280 (3)
N1—N2	1.408 (3)	N1B—N2B	1.404 (3)
N2—C2′	1.324 (3)	N2B—C2′B	1.324 (3)
N2—C3	1.514 (3)	N2B—C3B	1.513 (3)
N3′—C2′	1.308 (3)	N3′B—C2′B	1.312 (3)
N3′—C4′	1.376 (3)	N3′B—C4′B	1.370 (3)
C4′—C5′	1.523 (4)	C4′B—C5′B	1.531 (3)
C5′—H5′1	0.9700	C5′B—H5′3	0.9700
C5′—H5′2	0.9700	C5′B—H5′4	0.9700
C3—C9	1.517 (3)	C3B—C8B	1.517 (3)

C3—C8	1.519 (3)	C3B—C9B	1.522 (3)
C3—C3A	1.556 (3)	C3B—C3AB	1.555 (3)
C3A—C7A	1.497 (3)	C3AB—C7AB	1.493 (3)
C3A—C4	1.517 (4)	C3AB—C4B	1.529 (4)
C3A—H3A	0.9800	C3AB—H3AB	0.9800
C4—C5	1.532 (4)	C4B—C5B	1.529 (4)
C4—H4A	0.9700	C4B—H4B1	0.9700
C4—H4B	0.9700	C4B—H4B2	0.9700
C5—C6	1.524 (4)	C5B—C6B	1.516 (4)
C5—H5A	0.9700	C5B—H5B1	0.9700
C5—H5B	0.9700	C5B—H5B2	0.9700
C6—C10	1.525 (4)	C6B—C10B	1.527 (4)
C6—C7	1.534 (4)	C6B—C7B	1.528 (3)
C6—H6	0.9800	C6B—H6B	0.9800
C7—C7A	1.493 (3)	C7B—C7AB	1.490 (3)
C7—H7A	0.9700	C7B—H7B1	0.9700
C7—H7B	0.9700	C7B—H7B2	0.9700
C9—H9A	0.9600	C9B—H9B1	0.9600
C9—H9B	0.9600	C9B—H9B2	0.9600
C9—H9C	0.9600	C9B—H9B3	0.9600
C8—H8A	0.9600	C8B—H8B1	0.9600
C8—H8B	0.9600	C8B—H8B2	0.9600
C8—H8C	0.9600	C8B—H8B3	0.9600
C10—H10A	0.9600	C10B—H10D	0.9600
C10—H10B	0.9600	C10B—H10E	0.9600
C10—H10C	0.9600	C10B—H10F	0.9600
C2′—S1′—C5′	88.45 (12)	C2′B—S1′B—C5′B	88.60 (12)
C7A—N1—N2	106.63 (19)	C7AB—N1B—N2B	107.21 (19)
C2′—N2—N1	117.31 (18)	C2′B—N2B—N1B	117.75 (19)
C2′—N2—C3	129.48 (19)	C2′B—N2B—C3B	128.74 (19)
N1—N2—C3	113.19 (17)	N1B—N2B—C3B	113.44 (18)
C2′—N3′—C4′	111.1 (2)	C2′B—N3′B—C4′B	111.5 (2)
N3′—C2′—N2	124.0 (2)	N3′B—C2′B—N2B	123.7 (2)
N3′—C2′—S1′	118.80 (18)	N3′B—C2′B—S1′B	118.70 (18)
N2—C2′—S1′	117.20 (17)	N2B—C2′B—S1′B	117.56 (17)
O6′—C4′—N3′	124.6 (2)	O6′B—C4′B—N3′B	125.0 (2)
O6′—C4′—C5′	120.6 (2)	O6′B—C4′B—C5′B	120.5 (2)
N3′—C4′—C5′	114.8 (2)	N3′B—C4′B—C5′B	114.5 (2)
C4′—C5′—S1′	106.73 (19)	C4′B—C5′B—S1′B	106.68 (18)
C4′—C5′—H5′1	110.4	C4′B—C5′B—H5′3	110.4
S1′—C5′—H5′1	110.4	S1′B—C5′B—H5′3	110.4
C4′—C5′—H5′2	110.4	C4′B—C5′B—H5′4	110.4
S1′—C5′—H5′2	110.4	S1′B—C5′B—H5′4	110.4
H5′1—C5′—H5′2	108.6	H5′3—C5′B—H5′4	108.6
N2—C3—C9	108.11 (18)	N2B—C3B—C8B	109.00 (19)
N2—C3—C8	111.76 (19)	N2B—C3B—C9B	110.36 (19)
C9—C3—C8	111.3 (2)	C8B—C3B—C9B	112.0 (2)

N2—C3—C3A	99.17 (17)	N2B—C3B—C3AB	99.81 (18)
C9—C3—C3A	114.7 (2)	C8B—C3B—C3AB	110.28 (19)
C8—C3—C3A	111.2 (2)	C9B—C3B—C3AB	114.7 (2)
C7A—C3A—C4	111.0 (2)	C7AB—C3AB—C4B	107.9 (2)
C7A—C3A—C3	102.81 (19)	C7AB—C3AB—C3B	103.32 (19)
C4—C3A—C3	119.2 (2)	C4B—C3AB—C3B	119.4 (2)
C7A—C3A—H3A	107.8	C7AB—C3AB—H3AB	108.6
C4—C3A—H3A	107.8	C4B—C3AB—H3AB	108.6
C3—C3A—H3A	107.8	C3B—C3AB—H3AB	108.6
C3A—C4—C5	110.1 (2)	C3AB—C4B—C5B	109.9 (2)
C3A—C4—H4A	109.6	C3AB—C4B—H4B1	109.7
C5—C4—H4A	109.6	C5B—C4B—H4B1	109.7
C3A—C4—H4B	109.6	C3AB—C4B—H4B2	109.7
C5—C4—H4B	109.6	C5B—C4B—H4B2	109.7
H4A—C4—H4B	108.2	H4B1—C4B—H4B2	108.2
C6—C5—C4	112.3 (2)	C6B—C5B—C4B	112.9 (3)
C6—C5—H5A	109.1	C6B—C5B—H5B1	109.0
C4—C5—H5A	109.1	C4B—C5B—H5B1	109.0
C6—C5—H5B	109.1	C6B—C5B—H5B2	109.0
C4—C5—H5B	109.1	C4B—C5B—H5B2	109.0
H5A—C5—H5B	107.9	H5B1—C5B—H5B2	107.8
C5—C6—C10	112.2 (3)	C5B—C6B—C10B	112.1 (2)
C5—C6—C7	110.2 (2)	C5B—C6B—C7B	110.5 (2)
C10—C6—C7	109.9 (2)	C10B—C6B—C7B	109.6 (2)
C5—C6—H6	108.1	C5B—C6B—H6B	108.2
C10—C6—H6	108.1	C10B—C6B—H6B	108.2
C7—C6—H6	108.1	C7B—C6B—H6B	108.2
C7A—C7—C6	111.4 (2)	C7AB—C7B—C6B	110.2 (2)
C7A—C7—H7A	109.4	C7AB—C7B—H7B1	109.6
C6—C7—H7A	109.4	C6B—C7B—H7B1	109.6
C7A—C7—H7B	109.4	C7AB—C7B—H7B2	109.6
C6—C7—H7B	109.4	C6B—C7B—H7B2	109.6
H7A—C7—H7B	108.0	H7B1—C7B—H7B2	108.1
N1—C7A—C7	123.6 (2)	N1B—C7AB—C7B	123.1 (2)
N1—C7A—C3A	116.2 (2)	N1B—C7AB—C3AB	115.9 (2)
C7—C7A—C3A	120.1 (2)	C7B—C7AB—C3AB	120.7 (2)
C3—C9—H9A	109.5	C3B—C9B—H9B1	109.5
C3—C9—H9B	109.5	C3B—C9B—H9B2	109.5
H9A—C9—H9B	109.5	H9B1—C9B—H9B2	109.5
C3—C9—H9C	109.5	C3B—C9B—H9B3	109.5
H9A—C9—H9C	109.5	H9B1—C9B—H9B3	109.5
H9B—C9—H9C	109.5	H9B2—C9B—H9B3	109.5
C3—C8—H8A	109.5	C3B—C8B—H8B1	109.5
C3—C8—H8B	109.5	C3B—C8B—H8B2	109.5
H8A—C8—H8B	109.5	H8B1—C8B—H8B2	109.5
C3—C8—H8C	109.5	C3B—C8B—H8B3	109.5
H8A—C8—H8C	109.5	H8B1—C8B—H8B3	109.5
H8B—C8—H8C	109.5	H8B2—C8B—H8B3	109.5

C6—C10—H10A	109.5	C6B—C10B—H10D	109.5
C6—C10—H10B	109.5	C6B—C10B—H10E	109.5
H10A—C10—H10B	109.5	H10D—C10B—H10E	109.5
C6—C10—H10C	109.5	C6B—C10B—H10F	109.5
H10A—C10—H10C	109.5	H10D—C10B—H10F	109.5
H10B—C10—H10C	109.5	H10E—C10B—H10F	109.5

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the thiazole ring S1′/N3′/C2′/C4′/C5′

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5′—H5′2···O6′*B*^{i}	0.97	2.43	3.304 (4)	150
C9—H9*B*···O6′*B*^{ii}	0.96	2.53	3.361 (3)	145
C5′*B*—H5′3···O6′^{iii}	0.97	2.44	3.361 (3)	159
C4*B*—H4*B*2···*Cg*1	0.96	2.93	3.737 (4)	141
C7*B*—H7*B*2···*Cg*1^{iv}	0.96	2.90	3.867 (4)	174

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