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(*Z*)-*N*′-(3-Ethyl-4-oxothiazolidin-2-ylidene)-2-[6-(4-methoxyphenyl)imidazo[2,1-*b*]thiazol-3-yl]acetohydrazide

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Keywords: crystal structure; thiazole ring; imidazole ring; imidazo[2,1-*b*][1,3]thiazole ring system; thiazolidine ring; hydrogen bonding.

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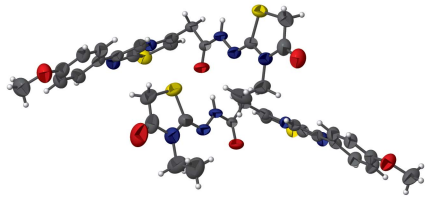
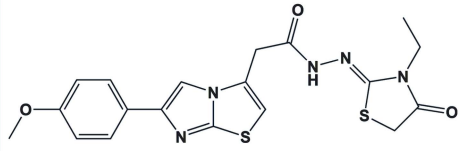
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{19}H_{19}N_5O_3S_2$, crystallizes in the triclinic space group $P\overline{1}$, with two independent molecules (*A* and *B*) in the asymmetric unit (Z' = 2). The imidazo[2,1-*b*][1,3]thiazole ring systems in molecules *A* and *B* are essentially planar (r.m.s deviations = 0.004 and 0.005 Å, respectively), with dihedral angles of 1.1 (3) and 0.8 (3)°, respectively, between the thiazole and imidazole rings. The mean planes of these ring systems make dihedral angles of 16.0 (2) and 61.9 (2)° for molecule *A*, and 11.8 (2) and 74.3 (2)° for molecule *B*, with the 1,3-thiazolidine and methoxy-substituted benzene rings, respectively. In the crystal, molecules are linked *via* N—H···O hydrogen bonds, forming –*A*–*B*–*A*–*B*– chains along [100]. The chains are linked by C—H···O hydrogen bonds, forming layers parallel to the *ab* plane.

3D view



Chemical scheme



Structure description

Continuing our work on the synthesis and crystal structure analyses of imidazo[2,1-*b*]thiazole derivatives (Akkurt *et al.*, 2007, 2008, 2011, 2012), we report herein on the synthesis and crystal structure of the title compound.

The asymmetric unit (Fig. 1) includes two crystallographically independent molecules (*A* and *B*). In molecules *A* and *B*, the thiazole and imidazole rings of the imidazo[2,1-*b*][1,3]thiazole group make dihedral angles of 1.1 (3) and 0.8 (3)°, respectively. The mean planes of the imidazo[2,1-*b*][1,3]thiazole ring systems make dihedral angles of 16.0 (2) and 61.9 (2)° for molecule *A*, and 11.8 (2) and 74.3 (2)° for molecule *B*, with the 1,3-

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···O5	0.86	1.99	2.758 (5)	148
N8—H8···O2^{i}	0.86	2.12	2.791 (5)	135
C17—H17···O2^{ii}	0.93	2.58	3.486 (6)	164
C28—H28···O4^{iii}	0.93	2.53	3.205 (7)	130

Symmetry codes: (i) $x+1, y, z$; (ii) $-x, -y+1, -z+2$; (iii) $x, y-1, z$.

thiazolidine ring and the methoxy-substituted benzene ring, respectively. The bond lengths and angles are comparable with the values reported for related structures (Akkurt *et al.*, 2007, 2008, 2011, 2012).

In the crystal, molecules are linked *via* N—H···O hydrogen bonds, forming *–A–B–A–B–* chains along [100]; see Table 1 and Fig. 2. The chains are linked by C—H···O hydrogen bonds, forming layers parallel to the *ab* plane; see Table 1 and Fig. 3.

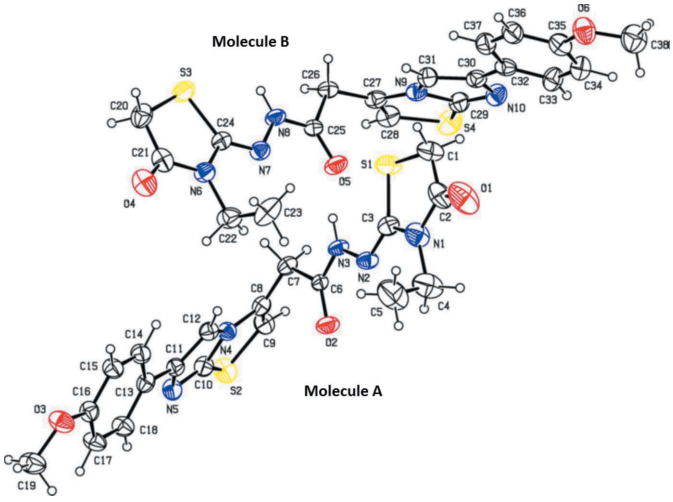


Figure 1
View of the molecular structure of the two independent molecules (*A* and *B*) of the title compound, with the atom labelling. Displacement ellipsoids are drawn at the 30% probability level.

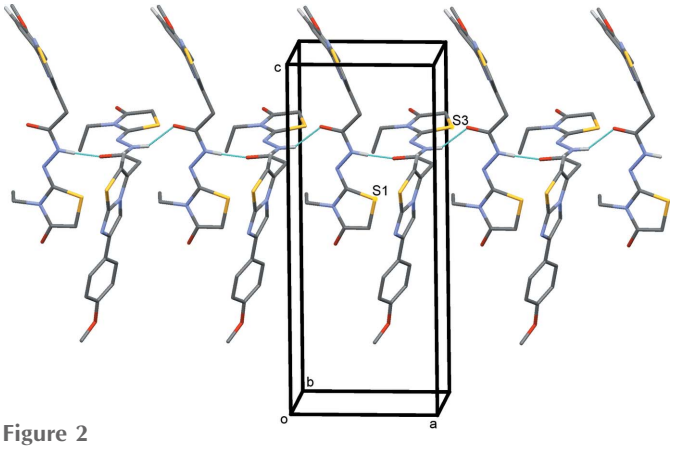


Figure 2
A partial view along the *b* axis of the crystal packing of the title compound. The chains propagating along [100] are generated by N—H···O hydrogen bonds (dashed lines; see Table 1).

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{19}H_{19}N_5O_3S_2$
M_r	429.51
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	296
a, b, c (Å)	8.2468 (6), 12.1136 (10), 19.8488 (17)
α, β, γ (°)	93.046 (4), 90.247 (4), 91.357 (4)
V (Å^3)	1979.5 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.30
Crystal size (mm)	0.12 × 0.07 × 0.06
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2007)
T_{min}, T_{max}	0.616, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	18894, 8167, 3286
R_{int}	0.090
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.629
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.069, 0.228, 0.95
No. of reflections	8167
No. of parameters	527
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.51, −0.38

Computer programs: *APEX2* and *SAINT* (Bruker, 2007), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *Mercury* (Macrae *et al.*, 2008), *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

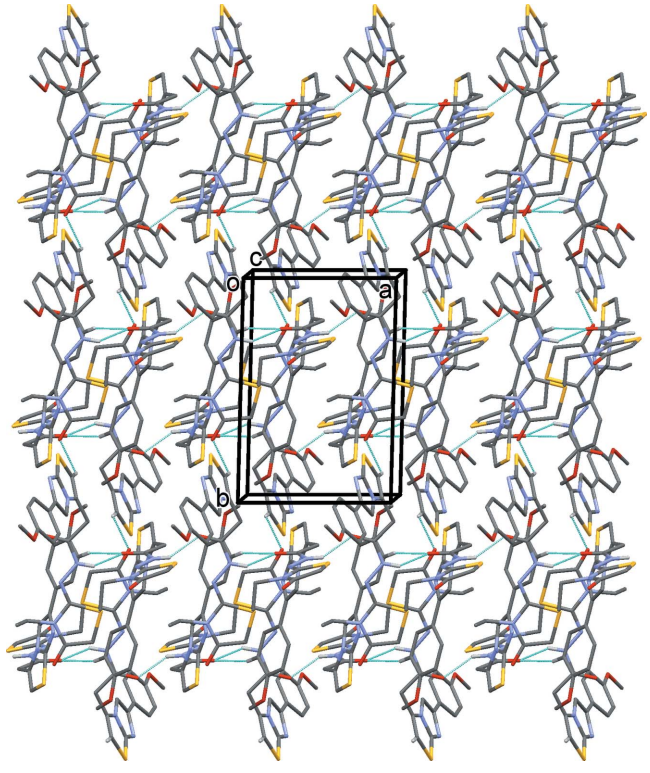


Figure 3
A view along the *c* axis of the crystal packing of the title compound. The N—H···O and C—H···O hydrogen bonds are shown as dashed lines (see Table 1).

Synthesis and crystallization

To a suspension of 4-ethyl-1-{[6-(4-methoxyphenyl)-imidazo[2,1-*b*][1,3]thiazol-3-yl]acetyl}-3-thiosemicarbazide (0.005 mol) in absolute ethanol (30 ml) were added anhydrous sodium acetate (0.02 mol) and ethyl bromoacetate (0.005 mol). The reaction mixture was refluxed for 5 h, then cooled, diluted with water and allowed to stand overnight. The solid that formed was filtered, dried and purified by crystallization from ethanol solution, yielding colourless prismatic crystals.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. A total of 15 reflections showing poor agreement between $|F_o|_2$ and $|F_c|_2$ were omitted in the final cycles of refinement.

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x170040 [https://doi.org/10.1107/S2414314617000402]

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Crystal data

$C_{19}H_{19}N_5O_3S_2$
M_r = 429.51
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 8.2468 (6) Å
b = 12.1136 (10) Å
c = 19.8488 (17) Å
α = 93.046 (4)°
β = 90.247 (4)°
γ = 91.357 (4)°
V = 1979.5 (3) Å^3
Z = 4
F(000) = 896
D_x = 1.441 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9344 reflections
θ = 3.0–24.1°
μ = 0.30 mm^{-1}
T = 296 K
Prism, colourless
0.12 × 0.07 × 0.06 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2007)
T_{min} = 0.616, T_{max} = 0.745
18894 measured reflections
8167 independent reflections
3286 reflections with $I > 2\sigma(I)$
R_{int} = 0.090
θ_{max} = 26.6°, θ_{min} = 3.0°
h = −10→10
k = −15→15
l = −24→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.228
S = 0.95
8167 reflections
527 parameters
1 restraint
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.106P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating -R-factor-obs etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.56576 (19)	0.29040 (13)	0.59729 (8)	0.0748 (6)
S2	0.2980 (2)	0.15834 (11)	1.02950 (7)	0.0668 (6)
S3	1.07508 (17)	0.51210 (12)	0.79043 (8)	0.0677 (6)
S4	0.7759 (2)	−0.18883 (11)	0.64921 (8)	0.0736 (6)
O1	0.2843 (7)	0.3964 (4)	0.4619 (2)	0.119 (2)
O2	0.2073 (4)	0.2551 (3)	0.80565 (16)	0.0637 (14)
O3	0.1369 (5)	0.9162 (3)	1.04151 (19)	0.0705 (16)
N1	0.2746 (6)	0.3555 (4)	0.5724 (2)	0.0751 (19)
N2	0.3077 (5)	0.3094 (3)	0.6832 (2)	0.0502 (16)
N3	0.4133 (4)	0.2754 (3)	0.73282 (19)	0.0460 (14)
N4	0.3520 (5)	0.3089 (3)	0.94710 (19)	0.0446 (12)
N5	0.2443 (5)	0.3890 (3)	1.0402 (2)	0.0534 (14)
C1	0.3506 (9)	0.3593 (5)	0.5105 (3)	0.082 (3)
C2	0.5184 (7)	0.3201 (5)	0.5122 (3)	0.079 (2)
C3	0.3696 (6)	0.3190 (4)	0.6249 (3)	0.0548 (19)
C4	0.0928 (9)	0.3776 (6)	0.5800 (3)	0.100 (3)
O4	0.7750 (5)	0.7480 (3)	0.82300 (19)	0.0767 (16)
C5	0.0812 (10)	0.4971 (7)	0.5968 (4)	0.125 (4)
O5	0.7088 (4)	0.1742 (3)	0.72153 (19)	0.0641 (14)
C6	0.3516 (6)	0.2519 (4)	0.7923 (2)	0.0416 (17)
O6	0.6582 (5)	0.1742 (3)	0.24916 (19)	0.0807 (17)
C7	0.4757 (6)	0.2185 (4)	0.8445 (2)	0.0492 (17)
C8	0.4040 (6)	0.2132 (4)	0.9122 (2)	0.0483 (17)
C9	0.3819 (6)	0.1257 (4)	0.9509 (2)	0.0587 (19)
C10	0.2936 (6)	0.2962 (4)	1.0101 (2)	0.0506 (17)
C11	0.2741 (6)	0.4672 (4)	0.9927 (2)	0.0458 (17)
C12	0.3411 (6)	0.4190 (4)	0.9354 (2)	0.0465 (17)
C13	0.2348 (6)	0.5834 (4)	1.0065 (2)	0.0462 (17)
C14	0.2983 (6)	0.6653 (4)	0.9667 (2)	0.0559 (19)
C15	0.2609 (6)	0.7743 (4)	0.9793 (3)	0.0553 (19)
C16	0.1616 (6)	0.8053 (4)	1.0322 (3)	0.0517 (17)
C17	0.0929 (6)	0.7253 (4)	1.0715 (3)	0.0591 (19)
C18	0.1311 (6)	0.6167 (4)	1.0574 (3)	0.0557 (19)
C19	0.0487 (8)	0.9542 (4)	1.0993 (3)	0.080 (3)
N6	0.7703 (5)	0.5647 (3)	0.7891 (2)	0.0547 (16)
N7	0.8079 (5)	0.3822 (3)	0.7555 (2)	0.0503 (14)
N8	0.9149 (5)	0.2966 (3)	0.7415 (2)	0.0505 (14)
N9	0.8507 (5)	0.0040 (3)	0.6115 (2)	0.0485 (14)
N10	0.7337 (5)	−0.0911 (3)	0.5234 (2)	0.0601 (17)

C20	1.0229 (7)	0.6496 (4)	0.8209 (3)	0.069 (2)
C21	0.8452 (8)	0.6619 (4)	0.8116 (3)	0.061 (2)
C22	0.5912 (7)	0.5534 (4)	0.7830 (3)	0.071 (2)
C23	0.5329 (8)	0.5701 (5)	0.7133 (4)	0.092 (3)
C24	0.8702 (6)	0.4756 (4)	0.7753 (2)	0.0478 (17)
C25	0.8537 (6)	0.1963 (4)	0.7252 (2)	0.0447 (17)
C26	0.9785 (6)	0.1079 (4)	0.7107 (2)	0.0492 (17)
C27	0.9019 (6)	0.0060 (4)	0.6789 (3)	0.0507 (19)
C28	0.8678 (6)	−0.0907 (4)	0.7055 (3)	0.062 (2)
C29	0.7803 (6)	−0.0934 (4)	0.5869 (3)	0.0548 (19)
C30	0.7759 (6)	0.0154 (4)	0.5056 (3)	0.0497 (19)
C31	0.8465 (6)	0.0738 (4)	0.5597 (2)	0.0507 (17)
C32	0.7420 (6)	0.0536 (4)	0.4386 (3)	0.0505 (17)
C33	0.6424 (7)	−0.0046 (4)	0.3937 (3)	0.064 (2)
C34	0.6102 (7)	0.0315 (4)	0.3305 (3)	0.066 (2)
C35	0.6791 (7)	0.1290 (4)	0.3116 (3)	0.063 (2)
C36	0.7777 (7)	0.1910 (4)	0.3562 (3)	0.066 (2)
C37	0.8090 (7)	0.1531 (4)	0.4188 (3)	0.063 (2)
C38	0.5680 (9)	0.1115 (6)	0.1995 (3)	0.097 (3)
H2A	0.59273	0.37650	0.49672	0.0950*
H2B	0.52834	0.25405	0.48278	0.0950*
H3	0.51543	0.26975	0.72511	0.0560*
H4A	0.03532	0.35732	0.53828	0.1200*
H4B	0.04670	0.33534	0.61571	0.1200*
H5A	0.13508	0.51529	0.63902	0.1870*
H5B	−0.03084	0.51629	0.60024	0.1870*
H5C	0.13184	0.53767	0.56196	0.1870*
H7A	0.51799	0.14683	0.83073	0.0590*
H7B	0.56562	0.27173	0.84638	0.0590*
H9	0.40915	0.05414	0.93667	0.0700*
H12	0.37251	0.45383	0.89679	0.0560*
H14	0.36681	0.64577	0.93115	0.0670*
H15	0.30306	0.82767	0.95177	0.0660*
H17	0.02268	0.74474	1.10644	0.0710*
H18	0.08438	0.56304	1.08346	0.0670*
H19A	−0.05373	0.91506	1.10044	0.1200*
H19B	0.03077	1.03194	1.09726	0.1200*
H19C	0.10970	0.94116	1.13934	0.1200*
H8	1.01813	0.30848	0.74349	0.0600*
H20A	1.05150	0.66091	0.86824	0.0830*
H20B	1.08185	0.70419	0.79591	0.0830*
H22A	0.54176	0.60718	0.81397	0.0850*
H22B	0.55705	0.48030	0.79579	0.0850*
H23A	0.55928	0.64433	0.70164	0.1370*
H23B	0.41749	0.55812	0.71106	0.1370*
H23C	0.58437	0.51878	0.68222	0.1370*
H26A	1.06087	0.13592	0.68085	0.0590*
H26B	1.03120	0.09053	0.75248	0.0590*

H28	0.89092	−0.10454	0.75009	0.0750*
H31	0.88415	0.14688	0.56082	0.0610*
H33	0.59478	−0.07075	0.40623	0.0760*
H34	0.54216	−0.00993	0.30093	0.0790*
H36	0.82268	0.25808	0.34399	0.0780*
H37	0.87628	0.19478	0.44860	0.0750*
H38A	0.61529	0.04029	0.19212	0.1460*
H38B	0.56900	0.14926	0.15820	0.1460*
H38C	0.45814	0.10237	0.21448	0.1460*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0560 (10)	0.0939 (11)	0.0755 (11)	0.0069 (8)	0.0148 (8)	0.0107 (9)
S2	0.0911 (12)	0.0498 (8)	0.0605 (9)	−0.0010 (7)	0.0056 (8)	0.0137 (6)
S3	0.0475 (9)	0.0672 (9)	0.0873 (11)	−0.0058 (7)	−0.0016 (8)	−0.0031 (8)
S4	0.0787 (11)	0.0529 (8)	0.0900 (12)	−0.0084 (7)	−0.0031 (9)	0.0161 (8)
O1	0.164 (5)	0.144 (4)	0.054 (3)	0.038 (4)	0.004 (3)	0.026 (3)
O2	0.035 (2)	0.101 (3)	0.056 (2)	0.0036 (19)	0.0010 (17)	0.0112 (19)
O3	0.085 (3)	0.052 (2)	0.075 (3)	0.006 (2)	0.026 (2)	0.0056 (18)
N1	0.082 (3)	0.094 (4)	0.051 (3)	0.016 (3)	−0.003 (3)	0.014 (3)
N2	0.038 (2)	0.061 (3)	0.053 (3)	0.0087 (19)	0.002 (2)	0.013 (2)
N3	0.026 (2)	0.061 (2)	0.052 (3)	0.0031 (18)	−0.001 (2)	0.011 (2)
N4	0.045 (2)	0.046 (2)	0.043 (2)	−0.0001 (19)	0.0017 (19)	0.0045 (19)
N5	0.065 (3)	0.048 (2)	0.047 (2)	−0.006 (2)	0.002 (2)	0.005 (2)
C1	0.112 (6)	0.085 (4)	0.049 (4)	0.007 (4)	0.011 (4)	0.005 (3)
C2	0.071 (4)	0.095 (4)	0.072 (4)	0.007 (4)	0.024 (3)	0.011 (3)
C3	0.048 (3)	0.055 (3)	0.062 (4)	0.002 (3)	0.000 (3)	0.009 (3)
C4	0.092 (3)	0.137 (6)	0.076 (5)	0.037 (5)	0.008 (4)	0.027 (4)
O4	0.108 (3)	0.050 (2)	0.073 (3)	0.004 (2)	0.007 (2)	0.0104 (19)
C5	0.134 (7)	0.151 (7)	0.091 (6)	0.041 (6)	0.005 (5)	0.003 (5)
O5	0.035 (2)	0.054 (2)	0.102 (3)	0.0026 (16)	0.0028 (19)	−0.0094 (19)
C6	0.031 (3)	0.047 (3)	0.046 (3)	0.003 (2)	−0.002 (2)	−0.006 (2)
O6	0.105 (3)	0.076 (3)	0.061 (3)	−0.004 (2)	−0.002 (2)	0.006 (2)
C7	0.037 (3)	0.055 (3)	0.056 (3)	0.002 (2)	−0.007 (2)	0.007 (2)
C8	0.044 (3)	0.050 (3)	0.051 (3)	−0.001 (2)	−0.008 (2)	0.005 (3)
C9	0.066 (4)	0.055 (3)	0.055 (3)	0.006 (3)	0.001 (3)	0.001 (3)
C10	0.055 (3)	0.051 (3)	0.046 (3)	−0.006 (3)	−0.001 (3)	0.009 (2)
C11	0.045 (3)	0.047 (3)	0.045 (3)	−0.006 (2)	0.002 (2)	0.002 (2)
C12	0.043 (3)	0.051 (3)	0.046 (3)	0.001 (2)	−0.001 (2)	0.008 (2)
C13	0.047 (3)	0.044 (3)	0.048 (3)	−0.006 (2)	−0.007 (3)	0.009 (2)
C14	0.062 (4)	0.055 (3)	0.050 (3)	−0.010 (3)	0.010 (3)	0.002 (3)
C15	0.066 (4)	0.047 (3)	0.053 (3)	−0.008 (3)	0.013 (3)	0.006 (2)
C16	0.059 (3)	0.044 (3)	0.052 (3)	−0.002 (3)	0.001 (3)	0.003 (2)
C17	0.065 (4)	0.057 (3)	0.056 (3)	0.002 (3)	0.021 (3)	0.007 (3)
C18	0.064 (4)	0.050 (3)	0.054 (3)	−0.002 (3)	0.012 (3)	0.012 (3)
C19	0.082 (5)	0.059 (4)	0.099 (5)	0.003 (3)	0.032 (4)	0.000 (3)
N6	0.049 (3)	0.046 (2)	0.069 (3)	0.005 (2)	0.002 (2)	0.001 (2)

N7	0.043 (2)	0.048 (2)	0.060 (3)	0.005 (2)	0.000 (2)	0.003 (2)
N8	0.029 (2)	0.052 (2)	0.070 (3)	0.005 (2)	0.001 (2)	−0.002 (2)
N9	0.044 (2)	0.044 (2)	0.058 (3)	0.0043 (19)	0.006 (2)	0.006 (2)
N10	0.061 (3)	0.049 (3)	0.070 (3)	−0.003 (2)	−0.002 (2)	0.002 (2)
C20	0.075 (4)	0.060 (3)	0.072 (4)	−0.018 (3)	−0.006 (3)	0.010 (3)
C21	0.085 (5)	0.047 (3)	0.052 (3)	0.003 (3)	0.004 (3)	0.011 (3)
C22	0.057 (4)	0.053 (3)	0.103 (5)	0.008 (3)	0.011 (3)	−0.002 (3)
C23	0.070 (4)	0.075 (4)	0.131 (6)	−0.012 (3)	−0.027 (4)	0.022 (4)
C24	0.042 (3)	0.051 (3)	0.051 (3)	0.000 (3)	−0.001 (2)	0.008 (2)
C25	0.034 (3)	0.050 (3)	0.050 (3)	0.007 (2)	0.001 (2)	−0.001 (2)
C26	0.037 (3)	0.055 (3)	0.056 (3)	0.007 (2)	0.004 (2)	0.004 (2)
C27	0.041 (3)	0.041 (3)	0.071 (4)	0.007 (2)	0.007 (3)	0.007 (3)
C28	0.059 (4)	0.055 (3)	0.074 (4)	0.006 (3)	0.001 (3)	0.011 (3)
C29	0.052 (3)	0.045 (3)	0.067 (4)	0.001 (2)	0.002 (3)	−0.001 (3)
C30	0.041 (3)	0.042 (3)	0.066 (4)	0.005 (2)	0.007 (3)	−0.001 (3)
C31	0.053 (3)	0.040 (3)	0.059 (3)	0.002 (2)	0.003 (3)	0.002 (3)
C32	0.045 (3)	0.045 (3)	0.062 (3)	0.011 (2)	0.011 (3)	0.003 (3)
C33	0.066 (4)	0.049 (3)	0.075 (4)	−0.003 (3)	−0.010 (3)	0.000 (3)
C34	0.070 (4)	0.060 (4)	0.067 (4)	−0.002 (3)	−0.009 (3)	0.000 (3)
C35	0.071 (4)	0.058 (3)	0.062 (4)	0.013 (3)	0.004 (3)	0.006 (3)
C36	0.074 (4)	0.061 (3)	0.061 (4)	−0.005 (3)	0.010 (3)	−0.001 (3)
C37	0.068 (4)	0.060 (3)	0.059 (4)	−0.005 (3)	0.005 (3)	−0.004 (3)
C38	0.102 (6)	0.115 (5)	0.075 (5)	0.010 (4)	−0.015 (4)	0.011 (4)

Geometric parameters (Å, º)

S1—C2	1.789 (6)	N7—C24	1.274 (6)
S1—C3	1.747 (5)	C7—H7B	0.9700
S2—C9	1.740 (4)	N7—N8	1.395 (5)
S2—C10	1.735 (5)	C7—H7A	0.9700
S3—C20	1.804 (5)	N8—C25	1.328 (6)
S3—C24	1.757 (5)	N9—C27	1.400 (7)
S4—C28	1.745 (6)	C9—H9	0.9300
S4—C29	1.737 (6)	N9—C29	1.368 (6)
O1—C1	1.219 (8)	N9—C31	1.366 (6)
O2—C6	1.221 (6)	N10—C29	1.318 (7)
O3—C19	1.423 (7)	N10—C30	1.392 (6)
O3—C16	1.367 (6)	C12—H12	0.9300
N1—C3	1.398 (7)	C14—H14	0.9300
N1—C4	1.536 (9)	C15—H15	0.9300
N1—C1	1.384 (8)	C17—H17	0.9300
N2—N3	1.397 (5)	C18—H18	0.9300
N2—C3	1.277 (7)	C19—H19B	0.9600
N3—C6	1.330 (6)	C19—H19C	0.9600
N4—C8	1.396 (6)	C19—H19A	0.9600
N4—C10	1.357 (6)	N8—H8	0.8600
N4—C12	1.371 (6)	C20—C21	1.488 (9)
N5—C11	1.390 (6)	C22—C23	1.488 (10)

N5—C10	1.318 (6)	C25—C26	1.520 (7)
C1—C2	1.474 (9)	C26—C27	1.483 (7)
N3—H3	0.8600	C27—C28	1.335 (7)
O4—C21	1.216 (7)	C30—C31	1.374 (7)
C4—C5	1.474 (11)	C30—C32	1.459 (8)
O5—C25	1.219 (6)	C32—C37	1.390 (7)
O6—C38	1.410 (8)	C32—C33	1.366 (8)
C6—C7	1.530 (6)	C33—C34	1.377 (8)
O6—C35	1.393 (7)	C34—C35	1.370 (7)
C7—C8	1.474 (6)	C35—C36	1.380 (8)
C8—C9	1.351 (6)	C36—C37	1.373 (8)
C11—C13	1.464 (7)	C20—H20A	0.9700
C11—C12	1.375 (6)	C20—H20B	0.9700
C13—C18	1.377 (7)	C22—H22A	0.9700
C13—C14	1.395 (7)	C22—H22B	0.9700
C14—C15	1.373 (7)	C23—H23A	0.9600
C15—C16	1.376 (8)	C23—H23B	0.9600
C16—C17	1.388 (7)	C23—H23C	0.9600
C17—C18	1.375 (7)	C26—H26A	0.9700
C2—H2B	0.9700	C26—H26B	0.9700
C2—H2A	0.9700	C28—H28	0.9300
C4—H4A	0.9700	C31—H31	0.9300
C4—H4B	0.9700	C33—H33	0.9300
C5—H5A	0.9600	C34—H34	0.9300
C5—H5B	0.9600	C36—H36	0.9300
C5—H5C	0.9600	C37—H37	0.9300
N6—C21	1.369 (7)	C38—H38A	0.9600
N6—C22	1.484 (7)	C38—H38B	0.9600
N6—C24	1.390 (6)	C38—H38C	0.9600

C2—S1—C3	92.6 (3)	C16—C15—H15	120.00
C9—S2—C10	89.6 (2)	C14—C15—H15	120.00
C20—S3—C24	91.5 (2)	C16—C17—H17	121.00
C28—S4—C29	89.8 (3)	C18—C17—H17	121.00
C16—O3—C19	118.2 (4)	C13—C18—H18	118.00
C1—N1—C4	121.4 (5)	C17—C18—H18	118.00
C1—N1—C3	115.5 (5)	H19B—C19—H19C	109.00
C3—N1—C4	122.8 (4)	H19A—C19—H19B	110.00
N3—N2—C3	115.6 (4)	H19A—C19—H19C	109.00
N2—N3—C6	118.2 (4)	O3—C19—H19A	109.00
C10—N4—C12	106.5 (4)	O3—C19—H19B	110.00
C8—N4—C12	137.2 (4)	O3—C19—H19C	109.00
C8—N4—C10	116.3 (4)	C25—N8—H8	121.00
C10—N5—C11	103.5 (4)	N7—N8—H8	121.00
O1—C1—N1	121.8 (6)	S3—C20—C21	108.3 (4)
O1—C1—C2	125.5 (6)	O4—C21—N6	124.1 (6)
N1—C1—C2	112.6 (5)	N6—C21—C20	112.0 (4)
S1—C2—C1	108.1 (4)	O4—C21—C20	123.9 (5)

N1—C3—N2	119.8 (5)	N6—C22—C23	112.3 (5)
C6—N3—H3	121.00	S3—C24—N7	128.9 (4)
S1—C3—N1	111.0 (4)	N6—C24—N7	119.7 (4)
S1—C3—N2	129.2 (4)	S3—C24—N6	111.4 (3)
N2—N3—H3	121.00	N8—C25—C26	115.1 (4)
N1—C4—C5	105.9 (6)	O5—C25—N8	123.9 (5)
O2—C6—N3	124.0 (4)	O5—C25—C26	121.0 (4)
N3—C6—C7	115.0 (4)	C25—C26—C27	111.2 (4)
O2—C6—C7	121.1 (4)	N9—C27—C28	110.5 (5)
C35—O6—C38	117.7 (4)	C26—C27—C28	129.6 (5)
C6—C7—C8	111.8 (4)	N9—C27—C26	119.9 (4)
N4—C8—C9	109.5 (4)	S4—C28—C27	114.1 (5)
N4—C8—C7	120.7 (4)	S4—C29—N10	136.7 (4)
C7—C8—C9	129.8 (4)	S4—C29—N9	110.1 (4)
S2—C9—C8	114.2 (4)	N9—C29—N10	113.3 (4)
S2—C10—N5	136.1 (3)	C31—C30—C32	128.1 (4)
S2—C10—N4	110.3 (3)	N10—C30—C32	122.0 (5)
N4—C10—N5	113.6 (4)	N10—C30—C31	109.9 (5)
N5—C11—C12	110.8 (4)	N9—C31—C30	106.9 (4)
C12—C11—C13	128.2 (4)	C33—C32—C37	117.5 (5)
N5—C11—C13	121.1 (4)	C30—C32—C33	122.1 (5)
N4—C12—C11	105.7 (4)	C30—C32—C37	120.4 (5)
C11—C13—C18	122.2 (4)	C32—C33—C34	122.1 (5)
C14—C13—C18	117.0 (4)	C33—C34—C35	119.5 (5)
C11—C13—C14	120.7 (4)	O6—C35—C36	114.8 (4)
C13—C14—C15	120.9 (4)	O6—C35—C34	125.3 (5)
C14—C15—C16	120.6 (5)	C34—C35—C36	119.9 (5)
C15—C16—C17	119.8 (5)	C35—C36—C37	119.6 (5)
O3—C16—C15	115.7 (5)	C32—C37—C36	121.3 (5)
O3—C16—C17	124.5 (5)	S3—C20—H20A	110.00
C16—C17—C18	118.4 (5)	S3—C20—H20B	110.00
C13—C18—C17	123.3 (5)	C21—C20—H20A	110.00
S1—C2—H2A	110.00	C21—C20—H20B	110.00
H2A—C2—H2B	108.00	H20A—C20—H20B	108.00
S1—C2—H2B	110.00	N6—C22—H22A	109.00
C1—C2—H2A	110.00	N6—C22—H22B	109.00
C1—C2—H2B	110.00	C23—C22—H22A	109.00
N1—C4—H4A	111.00	C23—C22—H22B	109.00
N1—C4—H4B	111.00	H22A—C22—H22B	108.00
C5—C4—H4A	111.00	C22—C23—H23A	109.00
H4A—C4—H4B	109.00	C22—C23—H23B	109.00
C5—C4—H4B	111.00	C22—C23—H23C	109.00
C4—C5—H5C	109.00	H23A—C23—H23B	109.00
H5A—C5—H5B	110.00	H23A—C23—H23C	109.00
H5B—C5—H5C	109.00	H23B—C23—H23C	109.00
C4—C5—H5A	110.00	C25—C26—H26A	109.00
H5A—C5—H5C	109.00	C25—C26—H26B	109.00
C4—C5—H5B	109.00	C27—C26—H26A	109.00

C22—N6—C24	121.6 (4)	C27—C26—H26B	109.00
C21—N6—C22	121.8 (4)	H26A—C26—H26B	108.00
C21—N6—C24	116.5 (4)	S4—C28—H28	123.00
C6—C7—H7A	109.00	C27—C28—H28	123.00
N8—N7—C24	116.9 (4)	N9—C31—H31	127.00
C6—C7—H7B	109.00	C30—C31—H31	127.00
C8—C7—H7A	109.00	C32—C33—H33	119.00
C8—C7—H7B	109.00	C34—C33—H33	119.00
H7A—C7—H7B	108.00	C33—C34—H34	120.00
N7—N8—C25	118.4 (4)	C35—C34—H34	120.00
C8—C9—H9	123.00	C35—C36—H36	120.00
C27—N9—C31	138.6 (4)	C37—C36—H36	120.00
S2—C9—H9	123.00	C32—C37—H37	119.00
C27—N9—C29	115.6 (4)	C36—C37—H37	119.00
C29—N9—C31	105.8 (4)	O6—C38—H38A	109.00
C29—N10—C30	104.1 (4)	O6—C38—H38B	109.00
N4—C12—H12	127.00	O6—C38—H38C	109.00
C11—C12—H12	127.00	H38A—C38—H38B	110.00
C13—C14—H14	120.00	H38A—C38—H38C	109.00
C15—C14—H14	120.00	H38B—C38—H38C	109.00

C3—S1—C2—C1	3.9 (4)	C11—C13—C18—C17	179.7 (5)
C2—S1—C3—N1	−3.2 (4)	C18—C13—C14—C15	1.5 (7)
C2—S1—C3—N2	175.8 (5)	C13—C14—C15—C16	1.0 (8)
C10—S2—C9—C8	−0.5 (4)	C14—C15—C16—C17	−2.8 (8)
C9—S2—C10—N4	0.7 (4)	C14—C15—C16—O3	177.9 (5)
C9—S2—C10—N5	178.4 (6)	C15—C16—C17—C18	2.1 (8)
C20—S3—C24—N7	−175.6 (4)	O3—C16—C17—C18	−178.6 (5)
C20—S3—C24—N6	3.2 (4)	C16—C17—C18—C13	0.4 (8)
C24—S3—C20—C21	−4.9 (4)	C22—N6—C21—C20	173.4 (5)
C28—S4—C29—N9	0.6 (4)	C24—N6—C21—C20	−3.6 (6)
C28—S4—C29—N10	−179.2 (6)	C24—N6—C22—C23	−86.9 (5)
C29—S4—C28—C27	−1.1 (4)	C22—N6—C24—S3	−177.4 (4)
C19—O3—C16—C15	−173.9 (5)	C24—N6—C21—O4	176.7 (5)
C19—O3—C16—C17	6.8 (8)	C22—N6—C24—N7	1.5 (6)
C3—N1—C1—C2	1.7 (7)	C21—N6—C24—N7	178.6 (4)
C1—N1—C3—N2	−177.7 (5)	C21—N6—C22—C23	96.2 (6)
C1—N1—C3—S1	1.4 (6)	C21—N6—C24—S3	−0.3 (5)
C4—N1—C1—O1	11.4 (9)	C22—N6—C21—O4	−6.2 (8)
C4—N1—C1—C2	−171.7 (5)	C24—N7—N8—C25	175.5 (4)
C4—N1—C3—S1	174.7 (4)	N8—N7—C24—N6	179.0 (4)
C3—N1—C1—O1	−175.2 (6)	N8—N7—C24—S3	−2.3 (6)
C4—N1—C3—N2	−4.4 (8)	N7—N8—C25—O5	0.2 (7)
C3—N1—C4—C5	95.6 (6)	N7—N8—C25—C26	180.0 (4)
C1—N1—C4—C5	−91.4 (6)	C31—N9—C29—S4	−179.1 (3)
N3—N2—C3—N1	−178.3 (4)	C31—N9—C29—N10	0.8 (6)
N3—N2—C3—S1	2.9 (7)	C29—N9—C27—C28	−0.7 (6)
C3—N2—N3—C6	−172.5 (4)	C27—N9—C29—N10	179.8 (4)

N2—N3—C6—C7	−178.3 (4)	C31—N9—C27—C28	177.8 (6)
N2—N3—C6—O2	2.2 (7)	C29—N9—C27—C26	−179.5 (4)
C8—N4—C10—N5	−179.1 (4)	C27—N9—C29—S4	−0.1 (5)
C12—N4—C8—C9	−179.0 (5)	C29—N9—C31—C30	−0.8 (5)
C10—N4—C8—C9	0.5 (6)	C31—N9—C27—C26	−0.9 (9)
C12—N4—C8—C7	3.0 (8)	C27—N9—C31—C30	−179.5 (6)
C10—N4—C12—C11	−0.6 (5)	C29—N10—C30—C32	−178.8 (5)
C10—N4—C8—C7	−177.5 (4)	C30—N10—C29—N9	−0.4 (6)
C8—N4—C10—S2	−0.9 (5)	C29—N10—C30—C31	−0.2 (5)
C8—N4—C12—C11	178.9 (5)	C30—N10—C29—S4	179.5 (5)
C12—N4—C10—S2	178.8 (3)	S3—C20—C21—N6	5.7 (6)
C12—N4—C10—N5	0.5 (6)	S3—C20—C21—O4	−174.7 (5)
C11—N5—C10—N4	−0.2 (5)	N8—C25—C26—C27	−167.6 (4)
C11—N5—C10—S2	−177.8 (5)	O5—C25—C26—C27	12.2 (6)
C10—N5—C11—C13	179.7 (4)	C25—C26—C27—N9	73.5 (5)
C10—N5—C11—C12	−0.2 (5)	C25—C26—C27—C28	−105.0 (6)
O1—C1—C2—S1	172.8 (5)	C26—C27—C28—S4	179.8 (4)
N1—C1—C2—S1	−3.9 (6)	N9—C27—C28—S4	1.2 (6)
C38—O6—C35—C34	−4.6 (8)	N10—C30—C32—C33	12.0 (8)
N3—C6—C7—C8	169.8 (4)	C31—C30—C32—C37	12.4 (8)
O2—C6—C7—C8	−10.8 (6)	N10—C30—C32—C37	−169.3 (5)
C38—O6—C35—C36	175.7 (5)	C31—C30—C32—C33	−166.4 (5)
C6—C7—C8—C9	115.9 (6)	N10—C30—C31—N9	0.7 (6)
C6—C7—C8—N4	−66.6 (6)	C32—C30—C31—N9	179.2 (5)
N4—C8—C9—S2	0.1 (5)	C30—C32—C37—C36	−179.5 (5)
C7—C8—C9—S2	177.9 (4)	C33—C32—C37—C36	−0.7 (8)
N5—C11—C13—C18	−17.2 (7)	C30—C32—C33—C34	179.9 (5)
N5—C11—C12—N4	0.5 (5)	C37—C32—C33—C34	1.1 (8)
C12—C11—C13—C18	162.7 (5)	C32—C33—C34—C35	−0.3 (9)
N5—C11—C13—C14	164.7 (4)	C33—C34—C35—C36	−1.1 (8)
C13—C11—C12—N4	−179.4 (5)	C33—C34—C35—O6	179.2 (5)
C12—C11—C13—C14	−15.4 (8)	O6—C35—C36—C37	−178.8 (5)
C14—C13—C18—C17	−2.1 (8)	C34—C35—C36—C37	1.5 (8)
C11—C13—C14—C15	179.6 (5)	C35—C36—C37—C32	−0.6 (9)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3···O5	0.86	1.99	2.758 (5)	148
N8—H8···O2^{i}	0.86	2.12	2.791 (5)	135
C17—H17···O2^{ii}	0.93	2.58	3.486 (6)	164
C28—H28···O4^{iii}	0.93	2.53	3.205 (7)	130

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