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Synthesis, crystal structure and Hirshfeld surface analysis of (*Z*)-2-({amino[6-phenyl-3-(4-methylphenyl)-1,2,4-triazin-5-yl]methylidene}amino)-6-methoxybenzo[*d*]thiazole-4,7-diyl diacetate

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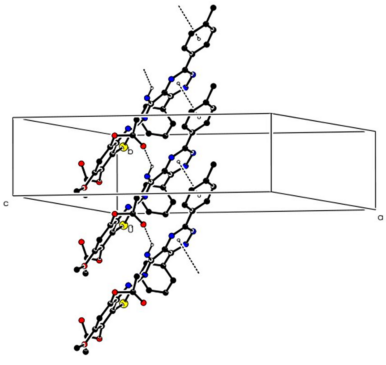
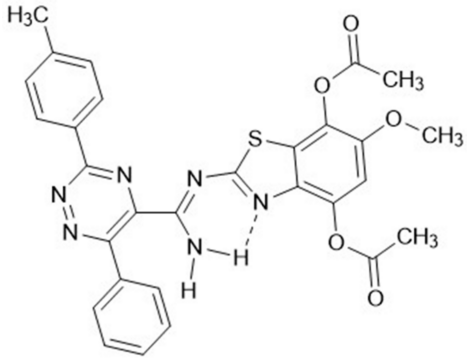
The stable conformation of the title molecule, $C_{29}H_{24}N_6O_5S$, is caused by two intramolecular N—H···N hydrogen bonds producing fused *S*(5) and *S*(6) rings. In the crystal, molecules are connected by intermolecular N—H···O interactions along the *b*-axis direction, forming *C*(9) chains. Furthermore, there are π–π interactions [centroid–to-centroid distance = 3.8200 (12) Å] between the benzene ring of the *p*-tolyl group and the 1,2,4-triazine ring in the same direction. As a result, the molecules form ribbons along the *b*-axis direction,. A Hirshfeld surface analysis was performed, showing the predominance of H···H, O···H/H···O, C···H/H···C and N···H/H···N contacts.

1. Chemical context

Metal-mediated or metal-free activation of nitriles (C≡N triple bonds) is a powerful synthetic strategy for the functionalization of organonitriles to form new N-heterocycles, ligands, metal complexes, catalysts, *etc*. (Kopylovich *et al.*, 2011; Mahmudov *et al.*, 2014). Recently, we developed a new synthetic method for functionalizing the C≡N nitrile group of 5-cyano-1,2,4-triazines with heterocyclic amines via a nucleophilic *ipso*-substitution reaction (Krinochkin *et al.*, 2022; Rammohan *et al.*, 2021); therefore, as a continuation of this work, we investigated 2-aminobenzothiazole as a nucleophile. It was found, that upon solvent-free interaction of 6-phenyl-3-(*p*-tolyl)-1,2,4-triazine-5-carbonitrile (**1**) with 6-methoxybenzo[*d*]thiazol-2-amine (**2**) at 423 K, the reaction yields the unexpected product (*Z*)-*N*′-(6-methoxybenzo[*d*]thiazol-2-yl)-6-phenyl-3-(*p*-tolyl)-1,2,4-triazine-5-carboximidamide (**3**). An attempt of oxidative cyclization of a six-membered intramolecular resonance-assisted hydrogen-bonding synthon (Mahmudov & Pombeiro, 2016) in (**3**) with lead tetraacetate in a benzene–acetic acid mixture (Mishra *et al.*, 2007) resulted in the diacylated product (*Z*)-2-({amino[6-phenyl-3-(*p*-tolyl)-1,2,4-triazin-5-yl]methylene}amino)-6-methoxybenzo[*d*]thiazole-4,7-diyl diacetate (**4**). The structures of the obtained compounds were confirmed by ^{1}H NMR spectroscopy, mass



spectrometry, and elemental analysis, as well as by single-crystal X-ray diffraction for compound (**4**).



2. Structural commentary

The title molecule (Fig. 1) has a stable conformation due to two intramolecular N—H···N hydrogen bonds that produce fused *S*(5) and *S*(6) rings (Table 1; Bernstein *et al.*, 1995). In a six-membered resonance-assisted hydrogen-bonding (RAHB) ring, the N3—H3*B*···N1 bond with [N···N distance = 2.676 (2) Å] falls in the N···N distance range [2.542–2.897 Å] observed for other supramolecular synthons (Gurbanov *et al.*, 2020), and indicates a low delocalization within the hetero-dienic moiety. The N—H···N angle of 130.8 (19)° differs significantly from the average O—H···O angle (149°; Bertolasi *et al.*, 1993) of *β*-diketone enols involved in similar intramolecular RAHB.

The 1,3-benzothiazole ring system (S1/N1/C1–C7) is essentially planar with a r.m.s. deviation of 0.0255 Å. The least-squares plane of this ring system forms angles of 17.2 (1), 81.2 (1), and 20.4 (1)° with the ring planes of the 1,2,4-triazine ring (N4–N6/C10–C12) and the benzene ring planes (C13–C18 and C20–C25) of its attached phenyl and 4-methylphenyl groups, respectively. The rings (C13–C18 and C20–C25) of the phenyl and 4-methylphenyl groups form angles of 62.1 (1)° with each other, while they make angles of 64.0 (1) and 5.8 (1)°, respectively, with the 1,2,4-triazine ring plane (N4–N6/C10–C12).

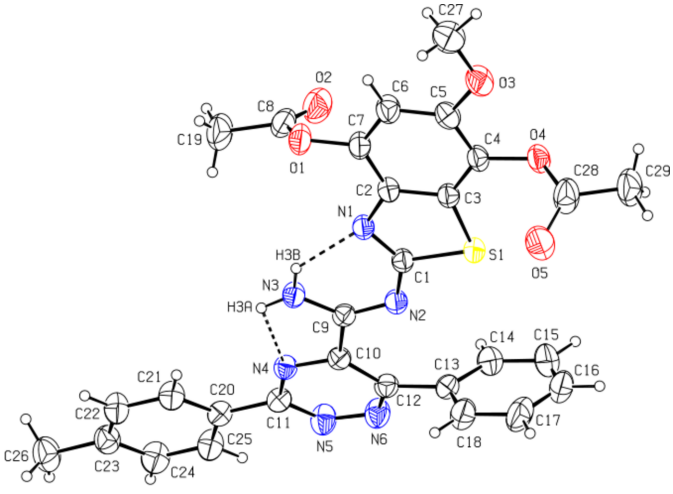


Figure 1
Molecular structure of the title compound showing the atomic labelling. Displacement ellipsoids are drawn at the 30% probability level.

3. Supramolecular features

In the crystal, the molecules, arranged at angles of approximately 45° to the *a*-axis direction and at equal intervals, are linked by intermolecular N—H···O interactions (Table 1) along the *b*-axis direction, forming *C*(9) chains. In addition, there are *π*-*π* interactions [*Cg*2···*Cg*5^{a} = 3.8200 (12) Å, shift = 1.107 Å and *Cg*5···*Cg*2^{b} = 3.8200 (12) Å, shift = 0.963 Å; symmetry codes (*a*) *x*, −1 + *y*, *z* and (*b*) x, 1 + *y*, *z*] between the

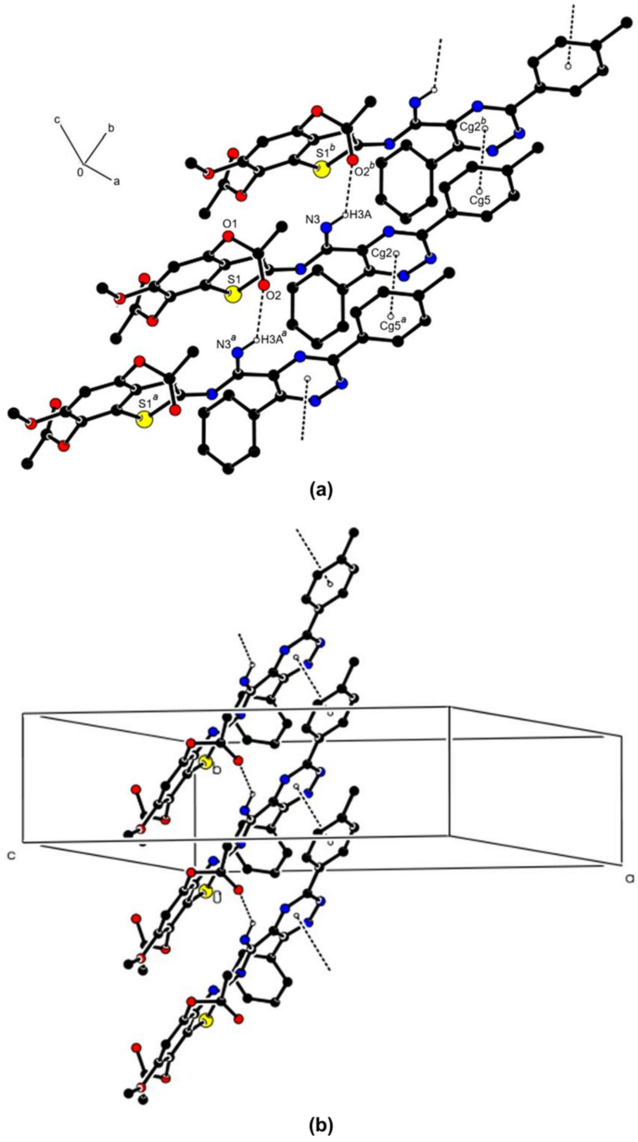


Figure 2
(*a*) Partial view of N—H···O hydrogen bonds and *π*–*π* interactions (dashed lines) in the unit cell of the title compound. H atoms not involved in hydrogen bonding and the minor component of the disordered O5 atom are omitted. (*b*) A different view of these interactions within a unit cell.

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···O2^{i}	0.87 (2)	2.59 (2)	3.229 (3)	130.5 (18)
N3—H3A···N4	0.87 (2)	2.23 (2)	2.613 (2)	106.8 (17)
N3—H3B···N1	0.93 (2)	1.97 (2)	2.676 (2)	130.8 (19)
C17—H17···O5^{ii}	0.93	2.55	3.390 (5)	150
C26—H26B···O2^{iii}	0.96	2.58	3.390 (4)	143
C27—H27A···O3^{iv}	0.96	2.53	3.389 (4)	150
C27—H27B···O5A^{v}	0.96	2.29	3.194 (8)	156

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

centroids *Cg*2 and *Cg*5 of the 1,2,4-triazine ring and the benzene ring of the *p*-tolyl group, along the *b*-axis direction (Fig. 2*a*,*b*). Thus, the molecules form ribbons along the *b*-axis direction. The cohesion of the packing is ensured by C—H···O interactions between these ribbons.

4. Hirshfeld surface analysis

A Hirshfeld surface analysis and the corresponding fingerprint plots were generated using *CrystalExplorer* software (Spackman *et al.*, 2021) to further investigate and quantify the contributions of the various intermolecular interactions in the crystal. The Hirshfeld surface mapped over d_{norm} using a fixed colour scale of −0.3005 (red) to 1.3598 (blue) a.u. and corresponding colours representing various interactions is shown in Fig. 3. The two-dimensional fingerprint plots for all intermolecular interactions and those delineated into specific contacts are shown in Fig. 4. The largest contribution comes from H···H contacts at 40.3% of the total, which is consistent with the significant hydrogen content of the molecule. The next most important contact is O···H/H···O at 20.1%, which primarily comes from the intramolecular O—H···O and intermolecular N—H···O as well as C—H···O interactions. The C···H/H···C interactions account for 15.4% while N···H/H···N contacts contribute 8.2%, followed by N···C/C···N contacts contributing 4.0%. Further, 3.9, 2.2, 1.2, 1.1, 0.5, 0.2 and 0.1% contributions corresponding to S···H/H···S, O···C/C···O, S···C/C···S, O···N/N···O, N···N, S···O/O···S and S···N/N···S contacts, respectively, are also observed.

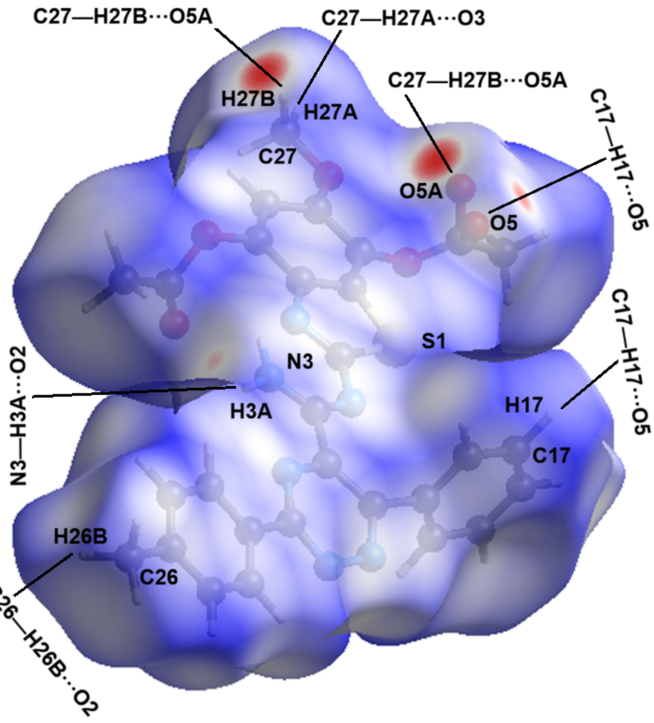


Figure 3
Hirshfeld surface of the title compound mapped over d_{norm}.

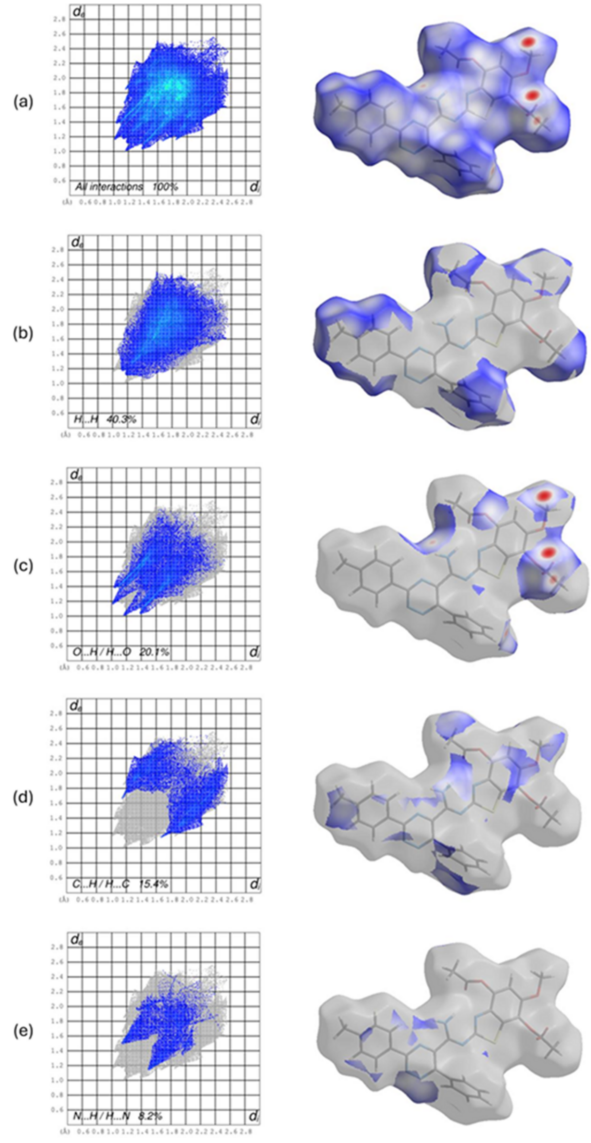


Figure 4
Hirshfeld surface mapped over d_{norm} and the corresponding two-dimensional fingerprint plots for the title compound. (*a*) All interactions (100%) and the relative contributions of (*b*) H···H (40.3%), (*c*) O···H/H···O (20.1%), (*d*) C···H/H···C (15.4%) and (*e*) N···H/H···N (8.2%) interactions to the Hirshfeld surface are indicated. The d_i and d_e values are the closest internal and external distances (in Å) from given points on the Hirshfeld surface.

5. Database survey

A search of the Cambridge Structural Database (CSD, Version 6.00, update of April 2025; Groom *et al.*, 2016) for the *N*′-(1,3-benzothiazol-2-yl)-1,2,4-triazine-5-carboximidamide unit generated six closely related compounds: (*Z*)-*N*-(4-methoxybenzo[*d*]thiazol-2-yl)-3,6-di-*p*-tolyl-1,2,4-triazine-5-carboximidamide (QARLOP: Shtaitz *et al.*, 2026), *N*-[(1,3-benzothiazol-2-yl)carbamothioyl]-4-bromobenzamide (JOMGOL: Sow *et al.*, 2024), *N*′-(1,3-benzothiazol-2-yl)benzenesulfonohydrazide (COCFOS: Baddeley *et al.*, 2019), *N*-(1,3-benzothiazol-2-yl)acetamide (TIJPAF: Nayak *et al.*, 2013), 2-[(6-methoxy-1,3-benzothiazol-2-yl)carbonoimidoyl]phenol (SUFFEG: Hijji *et al.*, 2015) and *N*-(4,6-dimethylpyrimidin-2-yl)-1,3-benzothiazol-2-amine (YAJBUI: Mohamed *et al.*, 2011).

QARLOP crystallizes in the triclinic $P\overline{1}$ space group while JOMGOL and YAJBUI crystallize in the monoclinic $P2_1/n$ space group. COCFOS has two molecules (*A* and *B*) in the asymmetric unit and crystallizes in the orthorhombic space group *Pbca*. TIJPAF has two molecules (*A* and *B*) in the asymmetric unit and crystallizes in the monoclinic space group $P2_1/c$. SUFFEG has two molecules in the asymmetric unit and crystallizes in the orthorhombic space group $Pna2_1$.

In the crystal of QARLOP, intermolecular C—H···O and C—H···N hydrogen bonds form layers parallel to the (010) plane. Furthermore, π–π and C—H···π [centroid-to-centroid distance = 3.7380 (12) Å] interactions connect molecules, forming ribbons along the *a*-axis direction. In JOMGOL, intermolecular C—H···N, C—H···S, and N—H···S hydrogen bonds form layers parallel to the *ac* plane. In YAJBUI, N—H···N hydrogen bonds link the molecules, generating a centrosymmetric cyclic hydrogen-bonded dimer with an $R_2^2(8)$ motif. In COCFOS, the *A* and *B* molecules in the asymmetric unit are linked into a supramolecular dimer via pairwise hydrazinyl-N—H···N(thiazolyl) hydrogen bonds. Hydrazinyl-N—H···O(sulfonyl) hydrogen bonds between *A* molecules assemble the dimers into chains along the *a*-axis direction, while links between centrosymmetrically related *B* molecules, leading to eight-membered $\{\cdots HNSO\}_2$ synthons, link the molecules along [001]. The result is an undulating supramolecular layer. Layers stack along the *b*-axis direction with benzothiazole-C—H···O(sulfonyl) points of contact being evident. In TIJPAF, the *A* and *B* molecules in the asymmetric unit are linked by N—H···N hydrogen-bond pairs, forming $R_2^2(8)$ dimer motifs along the [100] axis. In SUFFEG, a pair of C—H···O bonds connects two molecules in the asymmetric unit with the ring motif $R_2^2(20)$. Weak intermolecular C—H···N interactions also link these dimers, forming sheets parallel to the *ab* plane.

6. Synthesis and crystallization

The starting compound 5-cyano-1,2,4-triazine was prepared according to a literature procedure (Kozhevnikov *et al.*, 2002), and a known synthetic procedure (Shtaitz *et al.*, 2026) was used in the synthesis of (**4**).

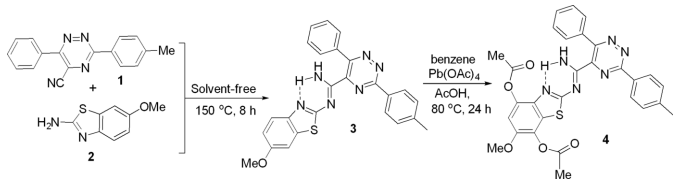


Figure 5
Reaction scheme for the title compound.

Synthesis of compound (3). 0.37 mmol of 6-phenyl-3-(*p*-tolyl)-1,2,4-triazine-5-carbonitrile (**1**) and 0.41 mmol of 6-methoxybenzo[*d*]thiazol-2-amine (**2**) were added into a round-bottom flask and the resulting mixture was heated at 423 K for 8 h under an inert atmosphere. The product was isolated by column chromatography (eluent AcOEt:$CDCl_3$ = 1:9; R_f 0.7 0.4). The pure product (*Z*)-*N*′-(6-methoxybenzo[*d*]-thiazol-2-yl)-6-phenyl-3-(*p*-tolyl)-1,2,4-triazine-5-carboximidamide (**3**) was obtained by recrystallization from ethanol solution. Yield 72 mg (43%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.48 (*s*, 3H, CH_3), 3.84 (*s*, 3H, OCH_3), 6.99–7.02 (*dd*, 1H, H-5 (benzothiazole), *J* 8.9 2.6 Hz,), 7.38–7.42 (*m*, 2H, $C_6H_4CH_3$), 7.45–7.50 (*m*, 3H, Ph), 7.56 (*br. s*, 1H, NH), 7.69–7.72 [*m*, 1H, H-4 (benzothiazole)], 7.77–7.80 (*m*, 2H, Ph), 8.49–8.53 (*m*, $C_6H_4CH_3$), 10.18 (*br. s*, 1H, NH). Mass-spectrum, *m*/*z* (I_{rel}, %): m/z: 453.15 $[M + H]^+$ (100). Found, %: C 66.34, H 4.44, N 18.58. $C_{25}H_{20}N_6OS$. Calculated, %: C 66.35, H 4.45, N 18.57.

Synthesis of compound (4): To a solution of 203 mg (0.45 mmol) of compound (**3**) in 15 mL of benzene and 5 mL of glacial acetic acid, 399 mg (0.90 mmol) of lead tetraacetate were added. The resulting mixture was stirred at 353 K for 24 h. The solvents were removed under reduced pressure (Fig. 5). The product was isolated by column chromatography (eluent AcOEt:$CDCl_3$ = 0.5:9.5; R_f 0.6). A single crystal of compound (**4**) was obtained by slow evaporation of a chloroform solution. (**4**): Yield 77 mg (30%). ^{1}H NMR (300 MHz, DMSO-d_6): δ = 2.34 (*s*, 3H, OAc), 2.43 (*s*, 3H, OAc), 2.48 (*s*, 3H, CH_3), 3.87 (*s*, 3H, OCH_3), 6.87 (*s*, 1H, H-5 (benzothiazole), 7.38–7.41 (*m*, 2H, $C_6H_4CH_3$), 7.45–7.52 (*m*, 3H, Ph), 7.69–7.77 (*m*, 3H, Ph+NH), 8.48–8.52 (*m*, $C_6H_4CH_3$), 9.99 (*br. s*, 1H, NH). Mass-spectrum, *m*/*z* (I_{rel}, %): *m*/*z*: 569.15 $[M+H]^+$ (100). Found, %: C 61.28, H 4.24, N 14.77. $C_{29}H_{24}N_6O_5S$. Calculated, %: C 61.26, H 4.25, N 14.78.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The H atoms of the NH_2 groups were found in difference-Fourier maps and were refined with $U_{iso}(H) = 1.2U_{eq}(N)$. The C-bound H atoms were positioned geometrically (C—H = 0.93–0.96 Å) and refined using a riding model, with $U_{iso}(H) = 1.2$ or $1.5U_{eq}(C)$. The oxygen atom (O5) of the carbonyl group exhibits disorder at two positions with a final occupancy ratio of 0.617 (4):0.383 (4). The disordered atom was modelled using SADI and EADP constraints.

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Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{29}H_{24}N_6O_5S$
M_r	568.60
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	293
a, b, c (Å)	19.7610 (5), 5.8264 (2), 24.3643 (5)
β (°)	94.711 (2)
V (Å^3)	2795.72 (13)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.17
Crystal size (mm)	0.41 × 0.25 × 0.16
Data collection	
Diffractometer	XtaLAB Synergy, Dualflex, HyPix
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2021)
T_{min}, T_{max}	0.951, 0.974
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	94505, 7321, 3876
R_{int}	0.094
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.695
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.052, 0.150, 1.04
No. of reflections	7321
No. of parameters	384
No. of restraints	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.21, −0.20

Computer programs: *CrysAlis PRO* (Rigaku OD, 2021), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2020).

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supporting information

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Synthesis, crystal structure and Hirshfeld surface analysis of (*Z*)-2-({amino[6-phenyl-3-(4-methylphenyl)-1,2,4-triazin-5-yl]methylidene}amino)-6-methoxybenzo[*d*]thiazole-4,7-diyl diacetate

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Computing details

(*Z*)-2-({Amino[6-phenyl-3-(4-methylphenyl)-1,2,4-triazin-5-yl]methylidene}amino)-6-methoxybenzo[*d*]thiazole-4,7-diyl diacetate

Crystal data

$C_{29}H_{24}N_6O_5S$
M_r = 568.60
Monoclinic, $P2_1/c$
a = 19.7610 (5) Å
b = 5.8264 (2) Å
c = 24.3643 (5) Å
β = 94.711 (2)°
V = 2795.72 (13) Å^3
Z = 4
$F(000)$ = 1184
D_x = 1.351 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 14058 reflections
θ = 1.7–22.1°
μ = 0.17 mm^{-1}
T = 293 K
Prism, red
0.41 × 0.25 × 0.16 mm

Data collection

XtaLAB Synergy, Dualflex, HyPix diffractometer
Radiation source: micro-focus sealed X-ray tube, PhotonJet (Mo) X-ray Source
Mirror monochromator
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2021)
T_{min} = 0.951, T_{max} = 0.974
94505 measured reflections
7321 independent reflections
3876 reflections with $I > 2\sigma(I)$
R_{int} = 0.094
θ_{max} = 29.6°, θ_{min} = 1.7°
h = −26→27
k = −8→8
l = −33→32

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.150
S = 1.04
7321 reflections
384 parameters
1 restraint
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0629P)^2 + 0.2039P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 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}	Occ. (<1)
C1	0.21371 (10)	−0.0169 (3)	0.37633 (8)	0.0501 (5)	
C2	0.17864 (10)	−0.2051 (3)	0.44712 (8)	0.0513 (5)	
C3	0.14532 (10)	−0.3400 (3)	0.40576 (8)	0.0506 (5)	
C4	0.10892 (10)	−0.5327 (3)	0.41903 (8)	0.0549 (5)	
C5	0.10454 (11)	−0.5896 (4)	0.47403 (9)	0.0634 (6)	
C6	0.13858 (12)	−0.4578 (4)	0.51514 (9)	0.0684 (6)	
H6	0.136281	−0.497031	0.551938	0.082*	
C7	0.17540 (11)	−0.2705 (4)	0.50151 (8)	0.0599 (5)	
C8	0.27976 (17)	−0.1373 (5)	0.54359 (10)	0.0828 (8)	
C9	0.27880 (10)	0.3049 (3)	0.36523 (8)	0.0482 (5)	
C10	0.31600 (10)	0.4545 (3)	0.32773 (7)	0.0486 (5)	
C11	0.39337 (10)	0.7418 (4)	0.32262 (8)	0.0526 (5)	
C12	0.31716 (10)	0.4223 (4)	0.27052 (8)	0.0536 (5)	
C13	0.27288 (12)	0.2688 (4)	0.23534 (8)	0.0579 (5)	
C14	0.30056 (15)	0.0875 (4)	0.20888 (10)	0.0819 (7)	
H14	0.347286	0.064348	0.212072	0.098*	
C15	0.2585 (2)	−0.0606 (5)	0.17743 (12)	0.1074 (11)	
H15	0.277110	−0.187109	0.160910	0.129*	
C16	0.1911 (2)	−0.0243 (6)	0.17039 (11)	0.1051 (10)	
H16	0.163484	−0.124743	0.149010	0.126*	
C17	0.16345 (16)	0.1595 (6)	0.19459 (11)	0.0970 (9)	
H17	0.117027	0.186958	0.189062	0.116*	
C18	0.20404 (13)	0.3049 (5)	0.22724 (10)	0.0787 (7)	
H18	0.184695	0.429212	0.244069	0.094*	
C19	0.30912 (18)	0.0520 (6)	0.57940 (12)	0.1174 (11)	
H19A	0.306157	0.193856	0.559294	0.176*	
H19B	0.355842	0.018822	0.590444	0.176*	
H19C	0.284211	0.065047	0.611465	0.176*	
C20	0.43176 (10)	0.9356 (4)	0.34862 (8)	0.0545 (5)	
C21	0.42356 (11)	0.9989 (4)	0.40250 (9)	0.0660 (6)	
H21	0.393252	0.918715	0.422600	0.079*	
C22	0.45978 (13)	1.1791 (4)	0.42650 (10)	0.0745 (7)	
H22	0.453821	1.217824	0.462820	0.089*	
C23	0.50483 (11)	1.3039 (4)	0.39798 (10)	0.0690 (6)	
C24	0.51209 (12)	1.2416 (4)	0.34442 (10)	0.0771 (7)	
H24	0.541801	1.323756	0.324156	0.093*	
C25	0.47656 (12)	1.0611 (4)	0.32009 (9)	0.0716 (6)	
H25	0.482770	1.022793	0.283793	0.086*	
C26	0.54425 (14)	1.5043 (5)	0.42390 (12)	0.0943 (8)	

H26A	0.571666	1.571426	0.397380	0.141*	
H26B	0.572946	1.451480	0.455052	0.141*	
H26C	0.513155	1.617094	0.435718	0.141*	
C27	0.06120 (16)	−0.8397 (5)	0.54036 (11)	0.0985 (9)	
H27A	0.036967	−0.981971	0.542078	0.148*	
H27B	0.036742	−0.720809	0.557540	0.148*	
H27C	0.105512	−0.855784	0.559273	0.148*	
C28	0.02414 (14)	−0.6465 (6)	0.35039 (12)	0.0957 (9)	
C29	0.00301 (16)	−0.8326 (5)	0.31195 (13)	0.1107 (11)	
H29A	0.036148	−0.850600	0.285579	0.166*	
H29B	−0.040186	−0.795503	0.293116	0.166*	
H29C	−0.000710	−0.973075	0.332058	0.166*	
N1	0.21598 (8)	−0.0226 (3)	0.42984 (6)	0.0517 (4)	
N2	0.24549 (8)	0.1299 (3)	0.34327 (6)	0.0532 (4)	
N3	0.28487 (9)	0.3671 (3)	0.41783 (7)	0.0552 (4)	
H3A	0.3075 (11)	0.491 (4)	0.4276 (9)	0.066*	
H3B	0.2614 (11)	0.277 (4)	0.4415 (9)	0.066*	
N4	0.35295 (8)	0.6197 (3)	0.35291 (6)	0.0510 (4)	
N5	0.40296 (10)	0.6934 (3)	0.27026 (7)	0.0698 (5)	
N6	0.36328 (10)	0.5355 (3)	0.24410 (7)	0.0698 (5)	
O1	0.20970 (9)	−0.1371 (3)	0.54256 (6)	0.0756 (5)	
O2	0.31015 (11)	−0.2704 (4)	0.51763 (9)	0.1052 (7)	
O3	0.06773 (9)	−0.7806 (3)	0.48390 (7)	0.0806 (5)	
O4	0.08296 (7)	−0.6852 (3)	0.37831 (6)	0.0671 (4)	
O5	0.0017 (2)	−0.4394 (7)	0.34761 (19)	0.1130 (14)	0.617 (4)
O5A	−0.0205 (3)	−0.5585 (12)	0.3785 (3)	0.1130 (14)	0.383 (4)
S1	0.16294 (3)	−0.23292 (9)	0.34217 (2)	0.05618 (17)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0507 (11)	0.0490 (11)	0.0500 (11)	0.0021 (9)	0.0011 (9)	−0.0068 (9)
C2	0.0538 (12)	0.0486 (11)	0.0514 (11)	−0.0045 (9)	0.0048 (9)	−0.0061 (9)
C3	0.0480 (11)	0.0484 (11)	0.0546 (11)	0.0008 (9)	−0.0008 (9)	−0.0062 (9)
C4	0.0505 (11)	0.0480 (12)	0.0650 (13)	−0.0035 (9)	−0.0036 (9)	−0.0115 (10)
C5	0.0621 (13)	0.0540 (13)	0.0746 (15)	−0.0123 (11)	0.0078 (11)	−0.0011 (11)
C6	0.0837 (16)	0.0635 (15)	0.0586 (13)	−0.0206 (12)	0.0094 (11)	−0.0043 (11)
C7	0.0716 (14)	0.0574 (13)	0.0507 (12)	−0.0142 (11)	0.0054 (10)	−0.0086 (10)
C8	0.106 (2)	0.084 (2)	0.0546 (14)	−0.0285 (17)	−0.0156 (14)	0.0050 (13)
C9	0.0467 (11)	0.0510 (12)	0.0470 (11)	0.0048 (9)	0.0034 (8)	−0.0007 (9)
C10	0.0474 (11)	0.0502 (11)	0.0482 (11)	0.0054 (9)	0.0049 (9)	−0.0010 (9)
C11	0.0492 (11)	0.0595 (13)	0.0497 (11)	−0.0002 (10)	0.0078 (9)	0.0014 (9)
C12	0.0573 (12)	0.0552 (12)	0.0484 (11)	0.0045 (10)	0.0060 (9)	−0.0005 (9)
C13	0.0744 (15)	0.0578 (13)	0.0412 (10)	−0.0001 (11)	0.0042 (10)	−0.0011 (9)
C14	0.109 (2)	0.0693 (17)	0.0663 (14)	0.0119 (15)	0.0009 (14)	−0.0127 (13)
C15	0.166 (3)	0.074 (2)	0.0796 (19)	0.007 (2)	−0.005 (2)	−0.0281 (15)
C16	0.153 (3)	0.090 (2)	0.0660 (17)	−0.030 (2)	−0.0258 (19)	−0.0088 (16)
C17	0.091 (2)	0.119 (3)	0.0759 (17)	−0.0212 (18)	−0.0224 (15)	−0.0093 (18)

C18	0.0767 (17)	0.0887 (19)	0.0687 (15)	−0.0005 (14)	−0.0063 (13)	−0.0146 (13)
C19	0.152 (3)	0.104 (2)	0.0905 (19)	−0.059 (2)	−0.0240 (18)	−0.0082 (17)
C20	0.0479 (11)	0.0624 (13)	0.0533 (12)	−0.0021 (10)	0.0048 (9)	0.0010 (10)
C21	0.0655 (14)	0.0714 (16)	0.0623 (13)	−0.0108 (12)	0.0122 (11)	−0.0041 (11)
C22	0.0804 (16)	0.0771 (17)	0.0664 (14)	−0.0115 (14)	0.0088 (12)	−0.0146 (12)
C23	0.0580 (13)	0.0686 (15)	0.0793 (16)	−0.0048 (11)	−0.0018 (12)	−0.0066 (12)
C24	0.0677 (15)	0.0888 (19)	0.0762 (16)	−0.0219 (14)	0.0147 (12)	−0.0011 (14)
C25	0.0703 (15)	0.0850 (17)	0.0605 (13)	−0.0202 (13)	0.0115 (11)	−0.0060 (12)
C26	0.0827 (18)	0.086 (2)	0.112 (2)	−0.0183 (15)	−0.0043 (15)	−0.0200 (16)
C27	0.114 (2)	0.087 (2)	0.096 (2)	−0.0385 (18)	0.0131 (17)	0.0159 (16)
C28	0.0722 (17)	0.100 (2)	0.109 (2)	0.0191 (16)	−0.0275 (15)	−0.0398 (18)
C29	0.099 (2)	0.100 (2)	0.126 (2)	−0.0037 (18)	−0.0388 (18)	−0.0402 (19)
N1	0.0569 (10)	0.0491 (10)	0.0489 (9)	−0.0057 (8)	0.0031 (7)	−0.0051 (7)
N2	0.0586 (10)	0.0508 (10)	0.0500 (9)	−0.0047 (8)	0.0038 (8)	−0.0033 (8)
N3	0.0621 (11)	0.0569 (11)	0.0469 (10)	−0.0117 (9)	0.0064 (8)	−0.0034 (8)
N4	0.0518 (9)	0.0542 (10)	0.0474 (9)	−0.0014 (8)	0.0066 (7)	−0.0017 (8)
N5	0.0754 (13)	0.0807 (14)	0.0555 (11)	−0.0163 (11)	0.0188 (10)	−0.0080 (10)
N6	0.0803 (13)	0.0765 (13)	0.0540 (10)	−0.0130 (11)	0.0133 (10)	−0.0072 (9)
O1	0.1031 (13)	0.0737 (11)	0.0502 (8)	−0.0307 (10)	0.0067 (8)	−0.0101 (7)
O2	0.0929 (14)	0.1154 (17)	0.1015 (15)	−0.0004 (12)	−0.0275 (12)	−0.0177 (13)
O3	0.0867 (12)	0.0673 (11)	0.0879 (12)	−0.0310 (9)	0.0085 (9)	0.0015 (9)
O4	0.0606 (9)	0.0546 (9)	0.0831 (10)	−0.0025 (7)	−0.0129 (8)	−0.0165 (7)
O5	0.092 (2)	0.085 (3)	0.152 (4)	0.026 (2)	−0.051 (2)	−0.031 (2)
O5A	0.092 (2)	0.085 (3)	0.152 (4)	0.026 (2)	−0.051 (2)	−0.031 (2)
S1	0.0613 (3)	0.0532 (3)	0.0525 (3)	−0.0023 (2)	−0.0044 (2)	−0.0077 (2)

Geometric parameters (Å, º)

C1—N1	1.301 (2)	C16—H16	0.9300
C1—N2	1.363 (2)	C17—C18	1.374 (4)
C1—S1	1.774 (2)	C17—H17	0.9300
C2—N1	1.380 (2)	C18—H18	0.9300
C2—C7	1.385 (3)	C19—H19A	0.9600
C2—C3	1.399 (3)	C19—H19B	0.9600
C3—C4	1.386 (3)	C19—H19C	0.9600
C3—S1	1.732 (2)	C20—C25	1.379 (3)
C4—C5	1.390 (3)	C20—C21	1.386 (3)
C4—O4	1.398 (2)	C21—C22	1.374 (3)
C5—O3	1.362 (2)	C21—H21	0.9300
C5—C6	1.391 (3)	C22—C23	1.381 (3)
C6—C7	1.368 (3)	C22—H22	0.9300
C6—H6	0.9300	C23—C24	1.373 (3)
C7—O1	1.397 (2)	C23—C26	1.512 (3)
C8—O2	1.193 (3)	C24—C25	1.372 (3)
C8—O1	1.383 (3)	C24—H24	0.9300
C8—C19	1.494 (4)	C25—H25	0.9300
C9—N2	1.305 (2)	C26—H26A	0.9600
C9—N3	1.328 (2)	C26—H26B	0.9600

C9—C10	1.498 (3)	C26—H26C	0.9600
C10—N4	1.328 (2)	C27—O3	1.434 (3)
C10—C12	1.408 (3)	C27—H27A	0.9600
C11—N5	1.335 (2)	C27—H27B	0.9600
C11—N4	1.336 (2)	C27—H27C	0.9600
C11—C20	1.474 (3)	C28—O5A	1.269 (7)
C12—N6	1.333 (3)	C28—O5	1.285 (4)
C12—C13	1.475 (3)	C28—O4	1.317 (3)
C13—C14	1.374 (3)	C28—C29	1.471 (4)
C13—C18	1.375 (3)	C29—H29A	0.9600
C14—C15	1.385 (4)	C29—H29B	0.9600
C14—H14	0.9300	C29—H29C	0.9600
C15—C16	1.346 (4)	N3—H3A	0.87 (2)
C15—H15	0.9300	N3—H3B	0.93 (2)
C16—C17	1.358 (4)	N5—N6	1.336 (3)

N1—C1—N2	128.96 (18)	C8—C19—H19C	109.5
N1—C1—S1	115.04 (15)	H19A—C19—H19C	109.5
N2—C1—S1	115.99 (14)	H19B—C19—H19C	109.5
N1—C2—C7	124.86 (17)	C25—C20—C21	117.8 (2)
N1—C2—C3	116.42 (17)	C25—C20—C11	121.24 (18)
C7—C2—C3	118.60 (18)	C21—C20—C11	120.99 (18)
C4—C3—C2	120.64 (18)	C22—C21—C20	120.6 (2)
C4—C3—S1	130.31 (16)	C22—C21—H21	119.7
C2—C3—S1	108.94 (15)	C20—C21—H21	119.7
C3—C4—C5	119.52 (18)	C21—C22—C23	121.6 (2)
C3—C4—O4	121.12 (18)	C21—C22—H22	119.2
C5—C4—O4	118.96 (18)	C23—C22—H22	119.2
O3—C5—C4	116.21 (19)	C24—C23—C22	117.4 (2)
O3—C5—C6	123.9 (2)	C24—C23—C26	120.7 (2)
C4—C5—C6	119.85 (19)	C22—C23—C26	121.9 (2)
C7—C6—C5	120.1 (2)	C25—C24—C23	121.6 (2)
C7—C6—H6	120.0	C25—C24—H24	119.2
C5—C6—H6	120.0	C23—C24—H24	119.2
C6—C7—C2	121.26 (19)	C24—C25—C20	121.0 (2)
C6—C7—O1	120.43 (18)	C24—C25—H25	119.5
C2—C7—O1	118.29 (18)	C20—C25—H25	119.5
O2—C8—O1	122.5 (2)	C23—C26—H26A	109.5
O2—C8—C19	127.0 (3)	C23—C26—H26B	109.5
O1—C8—C19	110.5 (3)	H26A—C26—H26B	109.5
N2—C9—N3	127.71 (18)	C23—C26—H26C	109.5
N2—C9—C10	117.43 (16)	H26A—C26—H26C	109.5
N3—C9—C10	114.85 (18)	H26B—C26—H26C	109.5
N4—C10—C12	120.05 (17)	O3—C27—H27A	109.5
N4—C10—C9	114.74 (16)	O3—C27—H27B	109.5
C12—C10—C9	125.09 (18)	H27A—C27—H27B	109.5
N5—C11—N4	123.62 (19)	O3—C27—H27C	109.5
N5—C11—C20	117.64 (17)	H27A—C27—H27C	109.5

N4—C11—C20	118.70 (17)	H27B—C27—H27C	109.5
N6—C12—C10	118.65 (19)	O5A—C28—O4	114.4 (4)
N6—C12—C13	114.57 (17)	O5—C28—O4	118.3 (3)
C10—C12—C13	126.76 (18)	O5A—C28—C29	117.9 (4)
C14—C13—C18	118.5 (2)	O5—C28—C29	125.5 (3)
C14—C13—C12	119.9 (2)	O4—C28—C29	113.3 (2)
C18—C13—C12	121.6 (2)	C28—C29—H29A	109.5
C13—C14—C15	119.6 (3)	C28—C29—H29B	109.5
C13—C14—H14	120.2	H29A—C29—H29B	109.5
C15—C14—H14	120.2	C28—C29—H29C	109.5
C16—C15—C14	121.0 (3)	H29A—C29—H29C	109.5
C16—C15—H15	119.5	H29B—C29—H29C	109.5
C14—C15—H15	119.5	C1—N1—C2	110.51 (16)
C15—C16—C17	119.9 (3)	C9—N2—C1	119.31 (16)
C15—C16—H16	120.1	C9—N3—H3A	119.6 (14)
C17—C16—H16	120.1	C9—N3—H3B	115.7 (13)
C16—C17—C18	120.0 (3)	H3A—N3—H3B	124.6 (19)
C16—C17—H17	120.0	C10—N4—C11	117.49 (16)
C18—C17—H17	120.0	C11—N5—N6	118.52 (17)
C17—C18—C13	120.8 (3)	C12—N6—N5	120.54 (17)
C17—C18—H18	119.6	C8—O1—C7	116.00 (18)
C13—C18—H18	119.6	C5—O3—C27	117.19 (18)
C8—C19—H19A	109.5	C28—O4—C4	120.97 (18)
C8—C19—H19B	109.5	C3—S1—C1	89.06 (9)
H19A—C19—H19B	109.5		

N1—C2—C3—C4	177.28 (18)	N4—C11—C20—C21	−3.5 (3)
C7—C2—C3—C4	1.1 (3)	C25—C20—C21—C22	−0.9 (3)
N1—C2—C3—S1	0.8 (2)	C11—C20—C21—C22	179.7 (2)
C7—C2—C3—S1	−175.45 (16)	C20—C21—C22—C23	0.6 (4)
C2—C3—C4—C5	1.2 (3)	C21—C22—C23—C24	0.1 (4)
S1—C3—C4—C5	176.86 (17)	C21—C22—C23—C26	179.2 (2)
C2—C3—C4—O4	−171.53 (18)	C22—C23—C24—C25	−0.6 (4)
S1—C3—C4—O4	4.2 (3)	C26—C23—C24—C25	−179.7 (2)
C3—C4—C5—O3	179.76 (19)	C23—C24—C25—C20	0.3 (4)
O4—C4—C5—O3	−7.4 (3)	C21—C20—C25—C24	0.4 (4)
C3—C4—C5—C6	−2.2 (3)	C11—C20—C25—C24	179.9 (2)
O4—C4—C5—C6	170.6 (2)	N2—C1—N1—C2	−177.39 (19)
O3—C5—C6—C7	178.9 (2)	S1—C1—N1—C2	1.7 (2)
C4—C5—C6—C7	1.0 (4)	C7—C2—N1—C1	174.3 (2)
C5—C6—C7—C2	1.3 (4)	C3—C2—N1—C1	−1.6 (2)
C5—C6—C7—O1	180.0 (2)	N3—C9—N2—C1	−2.1 (3)
N1—C2—C7—C6	−178.2 (2)	C10—C9—N2—C1	176.82 (17)
C3—C2—C7—C6	−2.3 (3)	N1—C1—N2—C9	−6.8 (3)
N1—C2—C7—O1	3.1 (3)	S1—C1—N2—C9	174.04 (14)
C3—C2—C7—O1	178.99 (18)	C12—C10—N4—C11	−3.8 (3)
N2—C9—C10—N4	−175.32 (17)	C9—C10—N4—C11	172.47 (16)
N3—C9—C10—N4	3.8 (2)	N5—C11—N4—C10	−6.2 (3)

N2—C9—C10—C12	0.8 (3)	C20—C11—N4—C10	176.25 (17)
N3—C9—C10—C12	179.85 (18)	N4—C11—N5—N6	9.7 (3)
N4—C10—C12—N6	10.2 (3)	C20—C11—N5—N6	−172.69 (19)
C9—C10—C12—N6	−165.74 (19)	C10—C12—N6—N5	−6.7 (3)
N4—C10—C12—C13	−171.40 (19)	C13—C12—N6—N5	174.70 (19)
C9—C10—C12—C13	12.7 (3)	C11—N5—N6—C12	−2.8 (3)
N6—C12—C13—C14	62.2 (3)	O2—C8—O1—C7	−12.1 (4)
C10—C12—C13—C14	−116.3 (2)	C19—C8—O1—C7	166.2 (2)
N6—C12—C13—C18	−116.5 (2)	C6—C7—O1—C8	114.8 (2)
C10—C12—C13—C18	65.1 (3)	C2—C7—O1—C8	−66.5 (3)
C18—C13—C14—C15	−3.5 (4)	C4—C5—O3—C27	−178.6 (2)
C12—C13—C14—C15	177.8 (2)	C6—C5—O3—C27	3.5 (4)
C13—C14—C15—C16	2.9 (5)	O5A—C28—O4—C4	−37.2 (6)
C14—C15—C16—C17	−0.3 (5)	O5—C28—O4—C4	22.3 (5)
C15—C16—C17—C18	−1.5 (5)	C29—C28—O4—C4	−176.2 (2)
C16—C17—C18—C13	0.8 (4)	C3—C4—O4—C28	−84.3 (3)
C14—C13—C18—C17	1.7 (4)	C5—C4—O4—C28	102.9 (3)
C12—C13—C18—C17	−179.6 (2)	C4—C3—S1—C1	−175.9 (2)
N5—C11—C20—C25	−0.7 (3)	C2—C3—S1—C1	0.18 (15)
N4—C11—C20—C25	177.1 (2)	N1—C1—S1—C3	−1.14 (16)
N5—C11—C20—C21	178.8 (2)	N2—C1—S1—C3	178.10 (16)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···O2^{i}	0.87 (2)	2.59 (2)	3.229 (3)	130.5 (18)
N3—H3*A*···N4	0.87 (2)	2.23 (2)	2.613 (2)	106.8 (17)
N3—H3*B*···N1	0.93 (2)	1.97 (2)	2.676 (2)	130.8 (19)
C17—H17···O5^{ii}	0.93	2.55	3.390 (5)	150
C21—H21···N4	0.93	2.52	2.830 (3)	100
C25—H25···N5	0.93	2.49	2.809 (3)	100
C26—H26*B*···O2^{iii}	0.96	2.58	3.390 (4)	143
C27—H27*A*···O3^{iv}	0.96	2.53	3.389 (4)	150
C27—H27*B*···O5*A*^{v}	0.96	2.29	3.194 (8)	156

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