

Crystal structure and Hirshfeld surface analysis of (benzo[4,5]imidazo[2,1-*b*]thiazol-2-yl)(4-chlorophenyl)methanone

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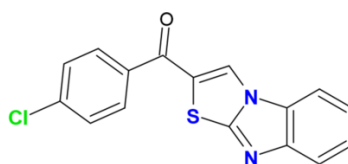
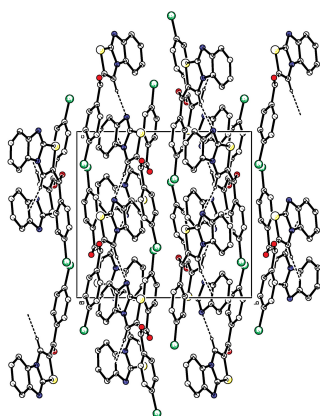
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Thiazolo[3,2-*a*]benzimidazole derivatives are biologically important heterocycles with diverse pharmacological activities such as anticancer and anti-inflammatory. The compound, C₁₆H₉ClN₂OS, crystallizes in the monoclinic space group *P*2₁/*c* with two conformationally similar molecules (*Z'* = 2) in the asymmetric unit. The fused thiazolo[3,2-*a*]benzimidazole framework is essentially planar, while the 4-chlorobenzoyl ring is inclined by ~53° to the thiazole ring in both molecules. The crystal packing is consolidated by C—H···N hydrogen bonds, C—H··· π contacts, and π – π stacking interactions, forming a three-dimensional supramolecular framework. Hirshfeld surface analysis indicates that H···H, H···C/C···H, H···Cl/Cl···H, H···N/N···H, and H···O/O···H contacts dominate the intermolecular interactions.

1. Chemical context

Benzimidazole is an important nitrogen-containing heterocyclic scaffold with a broad spectrum of biological activities, including anticancer, antimicrobial, and anti-inflammatory properties (Anichina *et al.*, 2017; Ramos Rodríguez *et al.*, 2019). Fusion with a thiazole ring affords thiazolo[3,2-*a*]benzimidazole derivatives, which often exhibit enhanced pharmacological profiles and have shown promise against cancer, HIV, and microbial infections (Al-Rashood & Abdel-Aziz, 2010; Khaldi *et al.*, 2020). Given that substitution patterns on the fused ring system significantly influence bioactivity, structural characterization by single-crystal X-ray diffraction is essential for establishing the molecular geometry and crystal packing, which are crucial for understanding structure–activity relationships (Ramos Rodríguez *et al.*, 2020). As part of our ongoing research on bioactive heterocycles (Al-Ansary *et al.*, 2017), we report the crystal structure of the title compound, C₁₆H₉ClN₂OS, (**3**).



2. Structural commentary

The title compound crystallizes in the monoclinic space group *P*2₁/*c* with two crystallographically independent molecules, *A* and *B*, in the asymmetric unit (Fig. 1). Both molecules share



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the same fused thiazolobenzimidazole core, comprising a thiazole ring (*B*), an imidazole ring (*C*), and a benzene ring (*D*), which adopts an essentially planar conformation in both independent molecules as observed in similar reported structures (Fun *et al.*, 2012*a,b*; Wang *et al.*, 2011). However, a comparative analysis reveals subtle differences in the degree of planarity between the two molecules: the interplanar angles between rings *B/C*, *C/D*, and *B/D* are 1.2 (2), 1.7 (1), and 2.7 (2)° for molecule *A*, compared to 1.0 (1), 0.8 (2), and 1.3 (2)° for molecule *B*, indicating that molecule *B* exhibits marginally greater coplanarity of the fused ring system, as further supported by the corresponding torsion angles (see the torsion angle table in the supporting information). In contrast, the 4-chlorobenzoyl substituents attached at the C9 position of the thiazole ring show a significant and remarkably similar deviation from the fused ring plane in both molecules, with dihedral angles between the 4-chlorophenyl ring (*A*) and the thiazole ring (*B*) of 53.0 (1)° for molecule *A* and 53.1 (3)° for molecule *B*, suggesting that this conformational preference is primarily governed by intrinsic electronic factors and steric avoidance rather than crystal packing influences. All bond lengths and bond angles (Table 1) in both molecules are within the expected ranges for analogous heterocyclic systems and show no statistically significant differences between the two independent molecules, confirming that molecules *A* and *B* are chemically equivalent but exhibit minor conformational

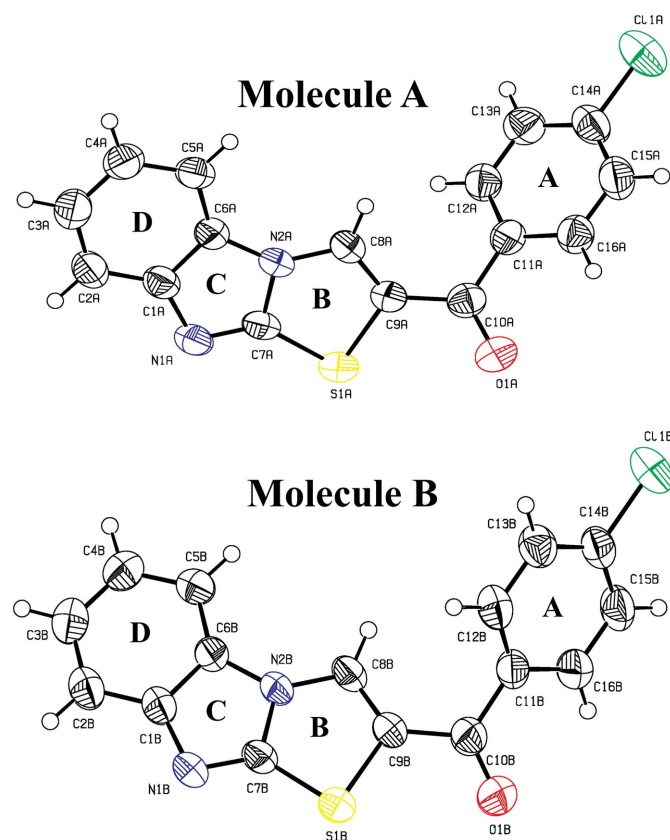


Figure 1
The molecular structures (molecules *A* and *B*) of compound **3** showing 50% displacement ellipsoids.

Table 1
Selected geometric parameters (Å, °).

S1B—C7B	1.725 (3)	N2A—C8A	1.375 (3)
S1B—C9B	1.760 (3)	N2A—C6A	1.390 (3)
S1A—C7A	1.726 (3)	O1A—C10A	1.220 (3)
S1A—C9A	1.762 (3)	N1B—C7B	1.305 (3)
N2B—C7B	1.382 (3)	N1B—C1B	1.404 (4)
N2B—C8B	1.370 (3)	O1B—C10B	1.219 (3)
N2B—C6B	1.393 (3)	N1A—C7A	1.305 (3)
N2A—C7A	1.383 (3)	N1A—C1A	1.407 (4)
C7B—S1B—C9B	89.83 (13)	N1B—C7B—N2B	114.3 (2)
C7A—S1A—C9A	89.93 (14)	C9B—C8B—N2B	112.2 (2)
C7B—N2B—C6B	106.8 (2)	C9A—C8A—N2A	112.7 (3)
C8B—N2B—C7B	114.8 (2)	C8B—C9B—S1B	112.4 (2)
C8B—N2B—C6B	138.4 (2)	C10B—C9B—S1B	120.1 (2)
C7A—N2A—C6A	106.7 (2)	N1B—C1B—C6B	111.8 (2)
C8A—N2A—C7A	114.4 (2)	C2B—C1B—N1B	129.5 (3)
C8A—N2A—C6A	138.9 (2)	C8A—C9A—S1A	112.2 (2)
C7B—N1B—C1B	103.4 (2)	C10A—C9A—S1A	119.9 (2)
C7A—N1A—C1A	103.4 (2)	N2B—C6B—C1B	103.8 (2)
N2A—C7A—S1A	110.8 (2)	C5B—C6B—N2B	132.5 (3)
N1A—C7A—S1A	135.0 (2)	N2A—C6A—C1A	104.1 (2)
N1A—C7A—N2A	114.2 (3)	C5A—C6A—N2A	132.0 (3)
N2B—C7B—S1B	110.7 (2)	C6A—C1A—N1A	111.6 (3)
N1B—C7B—S1B	135.0 (2)	C2A—C1A—N1A	129.8 (3)

Table 2
Hydrogen-bond geometry (Å, °).

Cg1, and Cg7 are the centroids of of atoms S1A/C7A/N2A/C8A/C9A and C1B—C6B, respectively.

D—H...A	D—H	H...A	D...A	D—H...A
C8A—H8A...N1A ⁱ	0.93	2.30	3.206 (3)	165
C8B—H8B...N1B ⁱⁱ	0.93	2.31	3.212 (3)	163
C13B—H13B...Cg1 ⁱⁱ	0.93	2.88	3.551 (4)	130
C16A—H16A...Cg7 ⁱⁱⁱ	0.93	3.00	3.832 (4)	150

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

variations, particularly in the planarity of the fused thiazolobenzimidazole core.

3. Supramolecular features and Hirshfeld surface analysis

Fig. 2 illustrates the packing of structure **3** along the crystallographic *a*-axis direction, wherein the overall cohesion of the unit cell is sustained by two intermolecular hydrogen bonds (Table 2; Fig. 3), C8A—H8A...N1A and C8B—H8B...N1B, that propagate into supramolecular chains parallel to the *c* axis. The crystal packing is characterized by weak C—H... π and aromatic π — π contacts (Fig. 4). The C13B—H13B...Cg1 and C16A—H16A...Cg7 contacts provide additional intermolecular links between neighbouring molecules. Several pairs of aromatic rings exhibit centroid-to-centroid separations in the range 3.731 (2)–4.011 (2) Å, namely Cg1...Cg3 = 3.731 (2) Å, Cg2...Cg3 = 4.011 (2) Å, Cg3...Cg4 = 3.748 (2) Å, Cg5...Cg7 = 3.893 (2) Å, Cg6...Cg7 = 3.924 (2) Å and Cg7...Cg8 = 3.787 (2) Å where Cg1, Cg2, Cg3 and Cg4 denote the centroids of the S1A/C7A/N2A/C8A/C9A, N1A/C1A/C6A/N2A/C7A, C11A—C16A and S1A/C7A/N1A/C1A/C6A/N2A/C8A/C9A ring systems, respectively, while Cg5, Cg6, Cg7 and Cg8 denote the corresponding centroids of

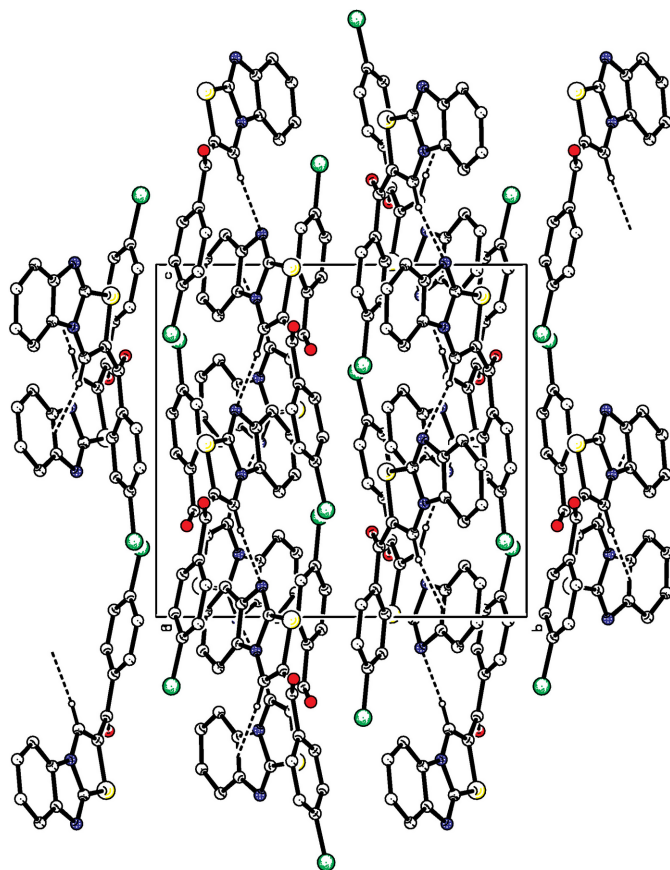


Figure 2
Packing diagram for compound **3** viewed down the *a* axis in the crystal unit cell. The dotted lines indicate the hydrogen bonds between symmetry-related molecules, which extend as C—H...N intermolecular interactions towards the *c*-axis direction in the unit-cell packing.

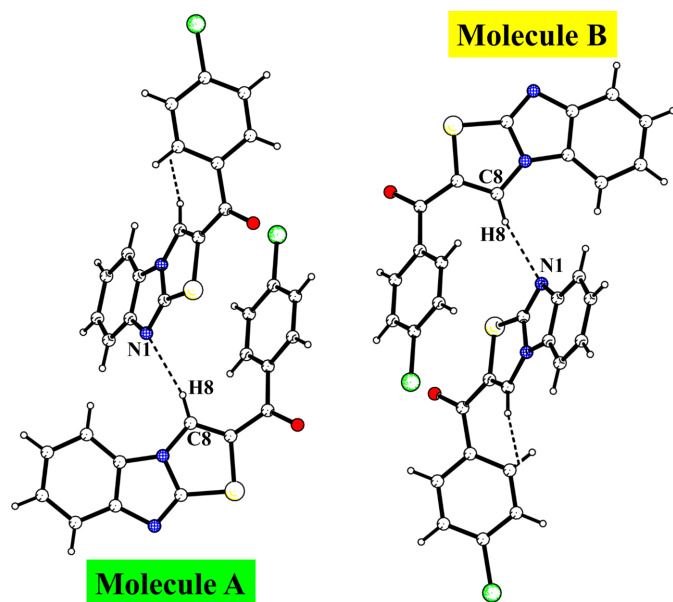


Figure 3
Hydrogen-bonding interactions in the crystal structure of compound **3**, showing the corresponding intermolecular contacts (C—H...N) involving the two crystallographically independent molecules **A** and **B**. Dashed lines indicate the hydrogen-bond interactions.

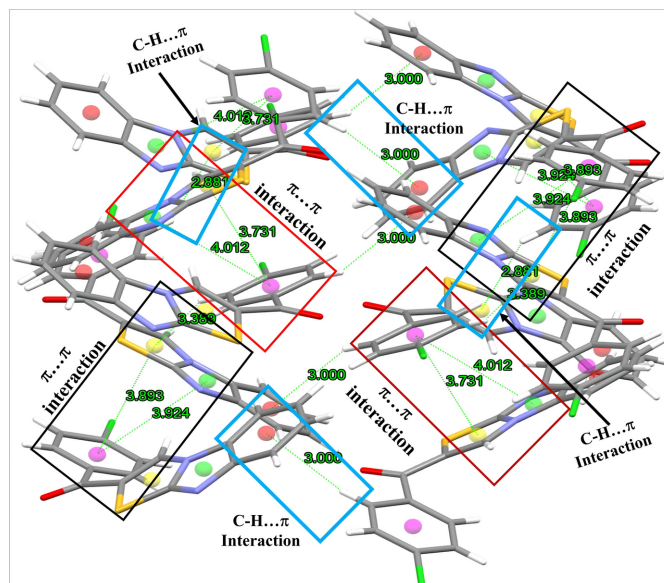


Figure 4
Visualization of intermolecular C—H... π (blue boxes) and π - π (red and black boxes) interactions in the crystal of compound **3**. Green dashed lines indicate interaction distances (Å).

the S1B/C7B/N2B/C8B/C9B, N1B/C1B/C6B/N2B/C7B, C1B–C6B and S1B/C7B/N1B/C1B/C6B/N2B/C8B/C9B ring systems. The Cg1...Cg3ⁱ, Cg3...Cg4ⁱ and Cg7...Cg8ⁱⁱ contacts are consistent with weak aromatic π – π associations (Fig. 4), while the Cg5...Cg7ⁱⁱ and Cg6...Cg7ⁱⁱ contacts, with slightly larger centroid-to-centroid separations, are indicative of weaker slipped or offset aromatic contacts [symmetry codes: (i) $x, \frac{1}{2} - y, \frac{1}{2} + z$; (ii) $x, \frac{3}{2} - y, -\frac{1}{2} + z$]. The Cg2...Cg3ⁱ separation of 4.011 (2) Å is comparatively long and is therefore regarded as a weak or borderline aromatic contact rather than a conventional π – π stacking interaction. Thus, the observed contacts are not interpreted as idealized face-to-face π – π stacks, but rather as a range of weak, slipped or offset aromatic associations arising from the relative disposition of the ring systems in the crystal. Together with the C–H... π contacts, these interactions contribute to the overall supramolecular organization of the crystal. Overall, these weak aromatic contacts, together with the other intermolecular

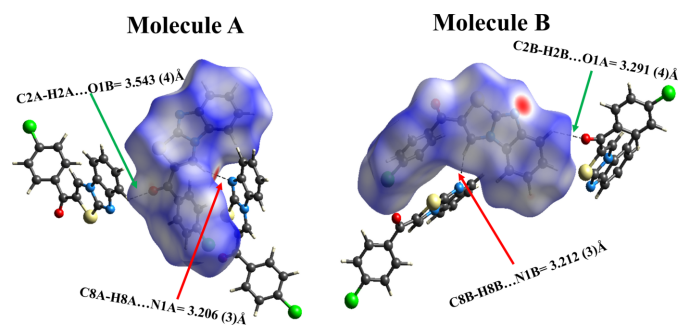


Figure 5
 Hirshfeld surface mapped with d_{norm} for compound **3**. Both molecules *A* and *B* form two types of intermolecular interactions, N—H...O and C—H...O, which contribute significantly to the cohesion of the crystal.

interactions present in the crystal, contribute to the cohesion and packing of the molecular structure.

The Hirshfeld surfaces (Fig. 5) and corresponding two-dimensional fingerprint plots (Fig. 4) of molecules *A* and *B* provide a comparative view of their intermolecular contacts and crystal-packing characteristics (Spackman *et al.*, 2021). In both molecules, the d_{norm} mapped surfaces show localized red regions associated with close intermolecular contacts, particularly around the heteroatom-containing sites. The Hirshfeld fingerprint analysis (Fig. 6) reveals closely comparable intermolecular contact distributions for the two independent molecules. For molecule *A*, the major contributions arise from C...H/H...C (21.4%), H...H (19.3%), Cl...H/H...Cl (13.0%), N...H/H...N (10.9%) and O...H/H...O (10.2%) contacts, while the corresponding contributions for molecule *B* are 22.8, 19.4, 10.7, 10.2 and 11.2%, respectively. The fingerprint plots are consistent with these values and show that C...H/H...C and H...H contacts constitute the principal contributions in both molecules. The short C8A—H8A...N1A [3.206 (3) Å] and C8B—H8B...N1B [3.212 (3) Å] contacts are consistent with the comparable N...H/H...N contributions. The O...H/H...O contribution is slightly higher for molecule *B*, consistent with the closer C—H...O contact observed for this molecule, whereas molecule *A* exhibits relatively larger Cl...H/H...Cl and S-associated contributions. Overall, the highly similar fingerprint profiles indicate comparable intermolecular contact environments for molecules *A* and *B*. The crystal packing is therefore consolidated by a cooperative combination of dispersive H...H, C...H/H...C and heteroatom-associated contacts, rather than by any single dominant interaction. The small differences in individual contact contributions reflect variations in the local

packing environments of the two crystallographically independent molecules.

4. Database survey

A systematic analysis of the Cambridge Structural Database (CSD, Version 5.47; Groom *et al.*, 2016), performed using the CCDC CONQUEST interface, was carried out to identify crystallographically characterized compounds structurally related to the title compound **3**. The search identified two closely related derivatives, namely benzo[4,5]imidazo[2,1-*b*]thiazol-2-yl(*p*-tolyl)methanone (CSD refcode ABESUY) and benzo[4,5]imidazo[2,1-*b*]thiazol-2-yl(4-fluorophenyl)methanone (ABESOS), reported by Ambethkar *et al.* (2017). These compounds contain *para*-methyl and *para*-fluoro substituents, respectively, on the phenyl ring of the benzoyl group. Their presence in the CSD provides useful structural precedents for assessing the influence of substitution on the conformation of the benzoyl-containing thiazolobenzimidazole framework.

The CSD search was subsequently extended to related compounds containing the thiazolo[3,2-*a*]benzimidazole core. Among the relevant structures, BACCUH (Chen *et al.*, 2020) and AMUCIW (Yallur *et al.*, 2016) are particularly useful for comparison. In these compounds, the benzoyl functionality is replaced by an aldehyde group; nevertheless, the principal geometrical characteristics and conformational features of the fused heteroaromatic framework are broadly comparable with those observed for compound **3**. Both structures also display aromatic π – π stacking interactions, indicating that such contacts may contribute significantly to the supramolecular organization of thiazolo[3,2-*a*]benzimidazole derivatives in the solid state. Further structural comparisons can be made

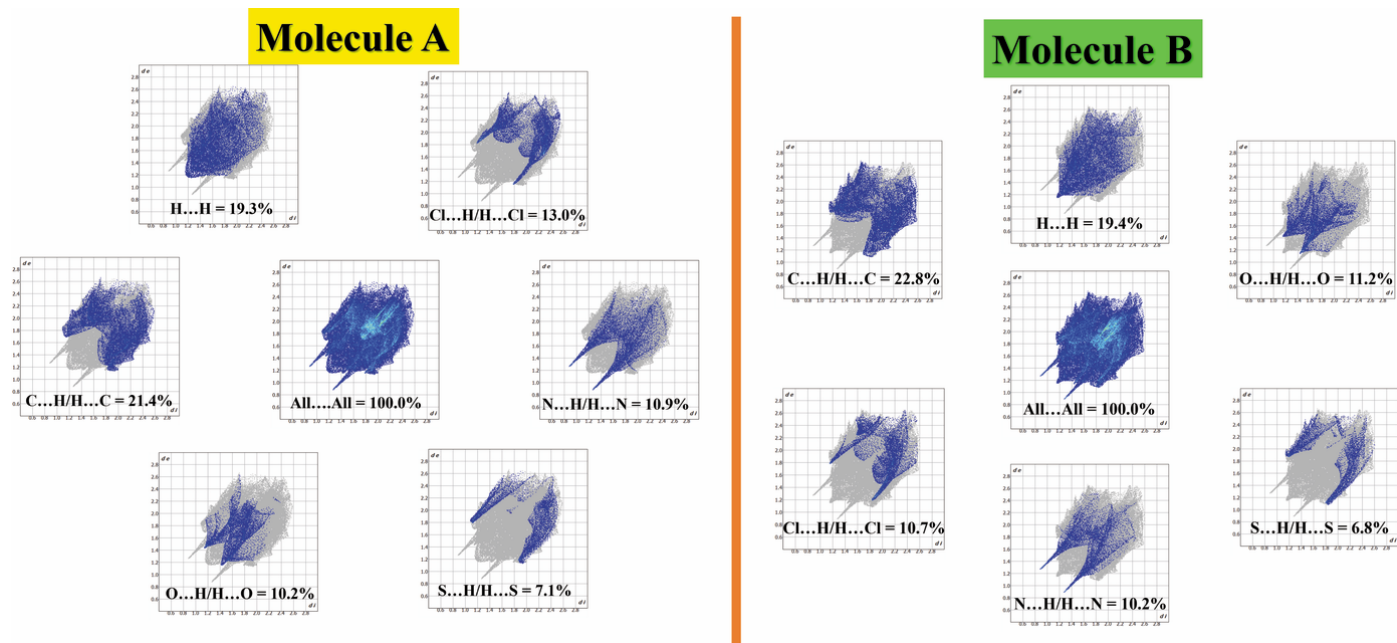


Figure 6

Hirshfeld surface fingerprint plots for compound **3** for molecules *A* and *B*. Contacts contributing >5% to the total surface are given with their respective percentage contributions labeled; those contributing less than 5% are shown in supplementary Figs. S1A and S1B.

with the benzoyl-containing CSD entries CANHEI (Zhang *et al.*, 2021) and CANHEI01 (Chen *et al.*, 2022). These structures possess an unsubstituted benzoyl group and exhibit geometrical parameters broadly consistent with those determined for compound **3**. The comparison suggests that modification of the peripheral substituents does not substantially alter the geometry of the fused thiazolo[3,2-*a*]benzimidazole skeleton, although differences in the orientation of the pendant phenyl ring can occur.

The methyl-ketone derivative FAQPAQ (Abdel-Aziz *et al.*, 2010) represents another structurally relevant example. In this compound, the thiazolo[3,2-*a*]benzimidazole unit adopts an essentially planar conformation and is associated with a pyrazolo[1,5-*a*]pyrimidine system. Although its overall molecular constitution differs from that of compound **3**, its nearly planar heteroaromatic framework supports the conformational preference observed for the corresponding core in the present structure. The reported biological activity of FAQPAQ, including its *in vitro* anticancer activity against colon cancer, further illustrates the continued interest in this heterocyclic scaffold. Other related structures, such as EXIVOX (Wang *et al.*, 2011) and QECZAB (Fun *et al.*, 2012b), provide additional insight into the intermolecular organization of this class of compounds. In EXIVOX, no significant classical intermolecular hydrogen-bonding interactions were reported, whereas the crystal packing of QECZAB is substantially influenced by π - π stacking interactions. These observations are consistent with the possibility that aromatic stacking and other weak intermolecular contacts can play an important role in consolidating the crystal packing of thiazolo[3,2-*a*]benzimidazole derivatives.

Overall, the CSD comparison indicates that the fused thiazolo[3,2-*a*]benzimidazole core generally favours an approximately planar geometry, consistent with its extended conjugated aromatic system. In compound **3**, however, attachment of the benzoyl substituent introduces an additional torsional degree of freedom, allowing the pendant phenyl ring to rotate with respect to the heteroaromatic core. The magnitude of this torsional deviation is likely governed by a combination of steric and electronic effects associated with the substituent on the phenyl ring. In particular, *para* substitution may influence both the preferred molecular conformation and the intermolecular packing arrangement. Thus, the structural features observed for compound **3**, including the planarity of the heteroaromatic core, the orientation of the benzoyl phenyl ring and the presence of π - π interactions, are broadly consistent with the structural trends evident from related thiazolo[3,2-*a*]benzimidazole derivatives reported in the CSD.

5. Synthesis and crystallization

A mixture of 1.0 equiv of 2-mercaptobenzimidazole (**1**), 1.0 equiv of (*E*)-1-(4-chlorophenyl)-3-(dimethylamino)prop-2-en-1-one (**2**), and 1.0 equiv of iodine in acetic acid (5 mL) was stirred at room temperature under open air for 2 h (Fig. 7). Upon completion (monitored by TLC), the reaction mixture was poured into water, quenched with aqueous sodium thio-

Table 3
Experimental details.

Crystal data	
Chemical formula	C ₁₆ H ₉ ClN ₂ OS
<i>M_r</i>	312.76
Crystal system, space group	Monoclinic, <i>P</i> ₂ ₁ / <i>c</i>
Temperature (K)	300
<i>a</i> , <i>b</i> , <i>c</i> (Å)	18.1878 (18), 12.8058 (13), 12.1917 (11)
β (°)	90.115 (4)
<i>V</i> (Å ³)	2839.6 (5)
<i>Z</i>	8
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.42
Crystal size (mm)	0.30 × 0.15 × 0.10
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015)
<i>T_{min}</i> , <i>T_{max}</i>	0.678, 0.746
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	94667, 7077, 3706
<i>R_{int}</i>	0.096
($\sin \theta/\lambda$) _{max} (Å ⁻¹)	0.668
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.059, 0.134, 1.11
No. of reflections	7077
No. of parameters	380
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	0.38, -0.33

Computer programs: *APEX3* (Bruker, 2016), *SAINT* (Bruker, 2017), *OLEX2.solve* (Bourhis *et al.*, 2015), *SHELXL2019/3* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

sulfate, and extracted with ethyl acetate. The combined organic layers were dried over Na₂SO₄ and concentrated under reduced pressure. The crude product, (benzo[4,5]-imidazo[2,1-*b*]thiazol-2-yl)(4-chlorophenyl)methanone (**3**) was purified by column chromatography and the well dried sample was crystallized using 100% ethylacetate as a solvent by slow evaporation method which yielded pale yellow crystal for diffraction study.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The carbon-bound hydrogen atoms were positioned based on calculated values (C—H = 0.93 Å) and were refined as riding atoms, with *U*_{iso}(H) set to 1.2*U*_{eq}(C).

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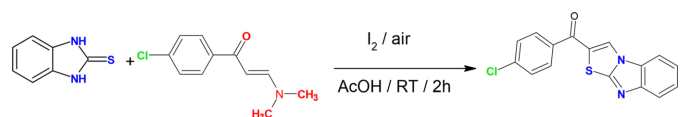


Figure 7
Synthetic route of the title compound (**3**).

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Crystal structure and Hirshfeld surface analysis of (benzo[4,5]imidazo[2,1-*b*]thiazol-2-yl)(4-chlorophenyl)methanone

R. Vishal, Vignesh Balaraman, Rajesh B. R. D. Yamajala and Sampath Natarajan

Computing details

(Benzo[4,5]imidazo[2,1-*b*]thiazol-2-yl)(4-chlorophenyl)methanone

Crystal data

C₁₆H₉ClN₂OS

$M_r = 312.76$

Monoclinic, $P2_1/c$

$a = 18.1878$ (18) Å

$b = 12.8058$ (13) Å

$c = 12.1917$ (11) Å

$\beta = 90.115$ (4)°

$V = 2839.6$ (5) Å³

$Z = 8$

$F(000) = 1280$

$D_x = 1.463$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 94667 reflections

$\theta = 2.0$ – 28.4°

$\mu = 0.42$ mm⁻¹

$T = 300$ K

Block, pale yellow

$0.30 \times 0.15 \times 0.10$ mm

Data collection

Bruker APEXII CCD

diffractometer

Radiation source: Mo $K\alpha$ (0.71073)

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(SADABS; Krause *et al.*, 2015)

$T_{\min} = 0.678$, $T_{\max} = 0.746$

94667 measured reflections

7077 independent reflections

3706 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.096$

$\theta_{\max} = 28.4^\circ$, $\theta_{\min} = 2.0^\circ$

$h = -24 \rightarrow 24$

$k = -17 \rightarrow 17$

$l = -16 \rightarrow 16$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.059$

$wR(F^2) = 0.134$

$S = 1.11$

7077 reflections

380 parameters

0 restraints

0 constraints

Primary atom site location: iterative

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0264P)^2 + 2.3482P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.38$ e Å⁻³

$\Delta\rho_{\min} = -0.33$ e Å⁻³

Extinction correction: SHELXL2019/2

(Sheldrick 2015),

$F_c^* = kFc[1 + 0.001x(Fc^2\lambda^3/\sin(2\theta))]^{-1/4}$

Extinction coefficient: 0.0031 (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 ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1B	0.15689 (4)	0.87765 (7)	0.91119 (6)	0.0579 (3)
S1A	0.34650 (4)	0.36471 (7)	0.99192 (6)	0.0572 (2)
Cl1B	0.13842 (6)	0.94112 (9)	0.21428 (7)	0.0852 (3)
Cl1A	0.37444 (7)	0.45888 (10)	0.30319 (8)	0.0999 (4)
N2B	0.26281 (12)	0.77668 (19)	0.82212 (16)	0.0444 (6)
N2A	0.23686 (13)	0.2692 (2)	0.90499 (17)	0.0474 (6)
O1A	0.46914 (12)	0.3712 (2)	0.82364 (18)	0.0708 (7)
N1B	0.27979 (13)	0.7804 (2)	1.00557 (17)	0.0505 (6)
O1B	0.03999 (13)	0.9172 (2)	0.74099 (18)	0.0804 (8)
N1A	0.21787 (14)	0.2853 (2)	1.08714 (18)	0.0532 (7)
C7A	0.26191 (16)	0.3049 (2)	1.0054 (2)	0.0480 (7)
C7B	0.23775 (15)	0.8083 (2)	0.9238 (2)	0.0466 (7)
C8B	0.21990 (16)	0.8074 (2)	0.7354 (2)	0.0496 (8)
H8B	0.230338	0.791704	0.662595	0.060*
C8A	0.28273 (16)	0.2910 (2)	0.8184 (2)	0.0492 (8)
H8A	0.272567	0.272234	0.746268	0.059*
C9B	0.16081 (16)	0.8629 (2)	0.7678 (2)	0.0483 (7)
C1B	0.33663 (16)	0.7245 (2)	0.9545 (2)	0.0482 (7)
C9A	0.34387 (16)	0.3422 (2)	0.8494 (2)	0.0496 (8)
C6B	0.32728 (15)	0.7205 (2)	0.8401 (2)	0.0455 (7)
C5A	0.12219 (17)	0.1675 (3)	0.8555 (2)	0.0548 (8)
H5A	0.130929	0.160840	0.780738	0.066*
C6A	0.17003 (16)	0.2200 (2)	0.9242 (2)	0.0474 (7)
C10B	0.09936 (17)	0.8982 (3)	0.6993 (2)	0.0540 (8)
C1A	0.15944 (16)	0.2308 (2)	1.0375 (2)	0.0499 (8)
C11B	0.11086 (16)	0.9082 (2)	0.5789 (2)	0.0498 (8)
C5B	0.37464 (17)	0.6696 (3)	0.7704 (2)	0.0554 (8)
H5B	0.366915	0.667852	0.694953	0.066*
C11A	0.39723 (16)	0.3855 (2)	0.6625 (2)	0.0482 (7)
C3B	0.44454 (18)	0.6231 (3)	0.9315 (3)	0.0605 (9)
H3B	0.485091	0.588914	0.961101	0.073*
C2A	0.09724 (17)	0.1867 (3)	1.0844 (3)	0.0578 (8)
H2A	0.088412	0.192151	1.159327	0.069*
C2B	0.39681 (17)	0.6737 (3)	1.0008 (3)	0.0574 (8)
H2B	0.404510	0.674055	1.076267	0.069*
C10A	0.40817 (17)	0.3665 (2)	0.7820 (2)	0.0524 (8)
C4B	0.43413 (17)	0.6213 (3)	0.8186 (3)	0.0590 (8)
H4B	0.468062	0.586749	0.774676	0.071*
C4A	0.06062 (17)	0.1256 (3)	0.9047 (3)	0.0612 (9)

H4A	0.026178	0.090667	0.861837	0.073*
C16A	0.45472 (17)	0.3662 (3)	0.5907 (3)	0.0582 (8)
H16A	0.498579	0.338939	0.617570	0.070*
C3A	0.04902 (18)	0.1345 (3)	1.0165 (3)	0.0620 (9)
H3A	0.007262	0.104148	1.046830	0.074*
C16B	0.05378 (17)	0.8820 (3)	0.5086 (2)	0.0589 (9)
H16B	0.009540	0.857925	0.537172	0.071*
C14B	0.12725 (19)	0.9288 (3)	0.3553 (2)	0.0562 (8)
C12B	0.17583 (18)	0.9459 (3)	0.5350 (3)	0.0584 (8)
H12B	0.214242	0.964260	0.581668	0.070*
C13B	0.18442 (18)	0.9566 (3)	0.4230 (3)	0.0597 (9)
H13B	0.228124	0.982144	0.394028	0.072*
C12A	0.33295 (17)	0.4283 (3)	0.6207 (3)	0.0567 (8)
H12A	0.294090	0.442577	0.667799	0.068*
C15B	0.06211 (18)	0.8912 (3)	0.3964 (3)	0.0635 (9)
H15B	0.024128	0.872187	0.349270	0.076*
C14A	0.3837 (2)	0.4293 (3)	0.4417 (3)	0.0624 (9)
C13A	0.32574 (19)	0.4500 (3)	0.5107 (3)	0.0613 (9)
H13A	0.282300	0.478202	0.483318	0.074*
C15A	0.44796 (19)	0.3868 (3)	0.4805 (3)	0.0684 (10)
H15A	0.486426	0.372046	0.432761	0.082*

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1B	0.0545 (5)	0.0800 (6)	0.0391 (4)	0.0107 (4)	0.0005 (3)	−0.0064 (4)
S1A	0.0545 (5)	0.0729 (6)	0.0441 (4)	−0.0056 (4)	−0.0096 (3)	−0.0040 (4)
Cl1B	0.1001 (8)	0.1075 (9)	0.0479 (5)	0.0073 (6)	−0.0047 (5)	0.0176 (5)
Cl1A	0.1188 (9)	0.1223 (10)	0.0586 (6)	−0.0032 (7)	0.0062 (6)	0.0263 (6)
N2B	0.0497 (14)	0.0530 (16)	0.0304 (11)	0.0036 (12)	−0.0023 (10)	−0.0024 (11)
N2A	0.0508 (15)	0.0585 (17)	0.0329 (12)	−0.0029 (12)	−0.0046 (10)	0.0018 (11)
O1A	0.0494 (13)	0.0950 (19)	0.0679 (15)	−0.0010 (13)	−0.0091 (11)	0.0039 (13)
N1B	0.0559 (15)	0.0625 (18)	0.0333 (12)	0.0021 (13)	−0.0019 (11)	0.0010 (12)
O1B	0.0607 (15)	0.125 (2)	0.0555 (14)	0.0245 (15)	−0.0010 (12)	−0.0075 (14)
N1A	0.0583 (16)	0.0636 (18)	0.0375 (13)	0.0015 (14)	−0.0052 (12)	0.0008 (12)
C7A	0.0531 (18)	0.055 (2)	0.0359 (15)	0.0030 (15)	−0.0086 (13)	0.0006 (14)
C7B	0.0499 (17)	0.057 (2)	0.0328 (14)	−0.0007 (15)	−0.0001 (12)	−0.0027 (14)
C8B	0.0564 (18)	0.061 (2)	0.0316 (14)	−0.0004 (16)	−0.0038 (13)	0.0019 (14)
C8A	0.0535 (18)	0.056 (2)	0.0380 (15)	−0.0022 (16)	0.0008 (13)	0.0014 (14)
C9B	0.0508 (17)	0.059 (2)	0.0351 (14)	0.0021 (16)	−0.0033 (13)	−0.0024 (14)
C1B	0.0518 (18)	0.051 (2)	0.0413 (16)	−0.0027 (15)	−0.0057 (13)	0.0030 (14)
C9A	0.0480 (18)	0.060 (2)	0.0402 (15)	0.0002 (15)	−0.0033 (13)	0.0003 (14)
C6B	0.0435 (16)	0.0521 (19)	0.0408 (15)	−0.0006 (15)	−0.0011 (12)	0.0050 (14)
C5A	0.059 (2)	0.062 (2)	0.0436 (16)	−0.0039 (17)	−0.0080 (14)	0.0015 (15)
C6A	0.0480 (17)	0.052 (2)	0.0418 (16)	−0.0041 (15)	−0.0020 (13)	0.0052 (14)
C10B	0.0536 (19)	0.063 (2)	0.0456 (17)	0.0052 (17)	−0.0051 (14)	−0.0062 (15)
C1A	0.0543 (19)	0.054 (2)	0.0416 (16)	0.0054 (16)	−0.0016 (14)	0.0051 (14)
C11B	0.0508 (18)	0.053 (2)	0.0458 (16)	0.0089 (15)	−0.0082 (14)	0.0001 (14)

C5B	0.060 (2)	0.062 (2)	0.0443 (16)	0.0053 (17)	0.0046 (15)	0.0020 (16)
C11A	0.0459 (17)	0.0456 (19)	0.0532 (17)	−0.0021 (14)	0.0010 (14)	−0.0008 (15)
C3B	0.0536 (19)	0.056 (2)	0.072 (2)	0.0004 (17)	−0.0110 (17)	0.0080 (18)
C2A	0.061 (2)	0.066 (2)	0.0459 (17)	0.0057 (18)	0.0063 (15)	0.0067 (16)
C2B	0.060 (2)	0.063 (2)	0.0490 (17)	−0.0053 (17)	−0.0116 (15)	0.0064 (16)
C10A	0.0501 (19)	0.052 (2)	0.0550 (18)	0.0032 (16)	−0.0030 (15)	−0.0015 (16)
C4B	0.0532 (19)	0.057 (2)	0.067 (2)	0.0048 (17)	0.0034 (16)	−0.0012 (17)
C4A	0.055 (2)	0.065 (2)	0.064 (2)	−0.0047 (18)	−0.0072 (16)	0.0036 (18)
C16A	0.0518 (19)	0.062 (2)	0.060 (2)	0.0036 (17)	0.0056 (15)	0.0036 (17)
C3A	0.0540 (19)	0.064 (2)	0.068 (2)	0.0002 (18)	0.0056 (17)	0.0080 (19)
C16B	0.0507 (18)	0.074 (2)	0.0519 (18)	0.0000 (17)	−0.0050 (15)	0.0032 (17)
C14B	0.066 (2)	0.056 (2)	0.0466 (17)	0.0067 (17)	−0.0092 (15)	0.0073 (16)
C12B	0.062 (2)	0.061 (2)	0.0527 (19)	−0.0036 (17)	−0.0145 (15)	0.0049 (16)
C13B	0.061 (2)	0.060 (2)	0.058 (2)	−0.0060 (17)	−0.0053 (16)	0.0117 (17)
C12A	0.0518 (19)	0.062 (2)	0.0559 (19)	0.0025 (16)	0.0046 (15)	0.0040 (17)
C15B	0.059 (2)	0.079 (3)	0.0525 (19)	−0.0017 (19)	−0.0197 (16)	0.0015 (18)
C14A	0.074 (2)	0.064 (2)	0.0491 (18)	−0.0061 (19)	0.0062 (17)	0.0084 (17)
C13A	0.063 (2)	0.057 (2)	0.064 (2)	0.0017 (17)	−0.0048 (17)	0.0090 (17)
C15A	0.065 (2)	0.079 (3)	0.061 (2)	0.000 (2)	0.0168 (17)	0.0056 (19)

Geometric parameters (Å, °)

S1B—C7B	1.725 (3)	C11B—C16B	1.386 (4)
S1B—C9B	1.760 (3)	C11B—C12B	1.385 (4)
S1A—C7A	1.726 (3)	C5B—H5B	0.9300
S1A—C9A	1.762 (3)	C5B—C4B	1.377 (4)
Cl1B—C14B	1.739 (3)	C11A—C10A	1.491 (4)
Cl1A—C14A	1.739 (3)	C11A—C16A	1.387 (4)
N2B—C7B	1.382 (3)	C11A—C12A	1.387 (4)
N2B—C8B	1.370 (3)	C3B—H3B	0.9300
N2B—C6B	1.393 (3)	C3B—C2B	1.376 (4)
N2A—C7A	1.383 (3)	C3B—C4B	1.389 (4)
N2A—C8A	1.375 (3)	C2A—H2A	0.9300
N2A—C6A	1.390 (3)	C2A—C3A	1.378 (4)
O1A—C10A	1.220 (3)	C2B—H2B	0.9300
N1B—C7B	1.305 (3)	C4B—H4B	0.9300
N1B—C1B	1.404 (4)	C4A—H4A	0.9300
O1B—C10B	1.219 (3)	C4A—C3A	1.384 (4)
N1A—C7A	1.305 (3)	C16A—H16A	0.9300
N1A—C1A	1.407 (4)	C16A—C15A	1.375 (4)
C8B—H8B	0.9300	C3A—H3A	0.9300
C8B—C9B	1.349 (4)	C16B—H16B	0.9300
C8A—H8A	0.9300	C16B—C15B	1.381 (4)
C8A—C9A	1.345 (4)	C14B—C13B	1.373 (4)
C9B—C10B	1.466 (4)	C14B—C15B	1.374 (4)
C1B—C6B	1.405 (4)	C12B—H12B	0.9300
C1B—C2B	1.392 (4)	C12B—C13B	1.382 (4)
C9A—C10A	1.464 (4)	C13B—H13B	0.9300

C6B—C5B	1.376 (4)	C12A—H12A	0.9300
C5A—H5A	0.9300	C12A—C13A	1.375 (4)
C5A—C6A	1.381 (4)	C15B—H15B	0.9300
C5A—C4A	1.380 (4)	C14A—C13A	1.375 (4)
C6A—C1A	1.402 (4)	C14A—C15A	1.372 (5)
C10B—C11B	1.488 (4)	C13A—H13A	0.9300
C1A—C2A	1.389 (4)	C15A—H15A	0.9300
C7B—S1B—C9B	89.83 (13)	C16A—C11A—C12A	118.3 (3)
C7A—S1A—C9A	89.93 (14)	C12A—C11A—C10A	122.3 (3)
C7B—N2B—C6B	106.8 (2)	C2B—C3B—H3B	118.9
C8B—N2B—C7B	114.8 (2)	C2B—C3B—C4B	122.1 (3)
C8B—N2B—C6B	138.4 (2)	C4B—C3B—H3B	118.9
C7A—N2A—C6A	106.7 (2)	C1A—C2A—H2A	121.0
C8A—N2A—C7A	114.4 (2)	C3A—C2A—C1A	117.9 (3)
C8A—N2A—C6A	138.9 (2)	C3A—C2A—H2A	121.0
C7B—N1B—C1B	103.4 (2)	C1B—C2B—H2B	121.1
C7A—N1A—C1A	103.4 (2)	C3B—C2B—C1B	117.8 (3)
N2A—C7A—S1A	110.8 (2)	C3B—C2B—H2B	121.1
N1A—C7A—S1A	135.0 (2)	O1A—C10A—C9A	120.2 (3)
N1A—C7A—N2A	114.2 (3)	O1A—C10A—C11A	121.2 (3)
N2B—C7B—S1B	110.7 (2)	C9A—C10A—C11A	118.6 (3)
N1B—C7B—S1B	135.0 (2)	C5B—C4B—C3B	121.4 (3)
N1B—C7B—N2B	114.3 (2)	C5B—C4B—H4B	119.3
N2B—C8B—H8B	123.9	C3B—C4B—H4B	119.3
C9B—C8B—N2B	112.2 (2)	C5A—C4A—H4A	119.3
C9B—C8B—H8B	123.9	C5A—C4A—C3A	121.4 (3)
N2A—C8A—H8A	123.7	C3A—C4A—H4A	119.3
C9A—C8A—N2A	112.7 (3)	C11A—C16A—H16A	119.4
C9A—C8A—H8A	123.7	C15A—C16A—C11A	121.1 (3)
C8B—C9B—S1B	112.4 (2)	C15A—C16A—H16A	119.4
C8B—C9B—C10B	127.1 (3)	C2A—C3A—C4A	122.2 (3)
C10B—C9B—S1B	120.1 (2)	C2A—C3A—H3A	118.9
N1B—C1B—C6B	111.8 (2)	C4A—C3A—H3A	118.9
C2B—C1B—N1B	129.5 (3)	C11B—C16B—H16B	119.7
C2B—C1B—C6B	118.7 (3)	C15B—C16B—C11B	120.5 (3)
C8A—C9A—S1A	112.2 (2)	C15B—C16B—H16B	119.7
C8A—C9A—C10A	127.4 (3)	C13B—C14B—C11B	118.8 (3)
C10A—C9A—S1A	119.9 (2)	C13B—C14B—C15B	121.6 (3)
N2B—C6B—C1B	103.8 (2)	C15B—C14B—C11B	119.6 (2)
C5B—C6B—N2B	132.5 (3)	C11B—C12B—H12B	119.5
C5B—C6B—C1B	123.8 (3)	C13B—C12B—C11B	121.0 (3)
C6A—C5A—H5A	122.1	C13B—C12B—H12B	119.5
C4A—C5A—H5A	122.1	C14B—C13B—C12B	118.8 (3)
C4A—C5A—C6A	115.9 (3)	C14B—C13B—H13B	120.6
N2A—C6A—C1A	104.1 (2)	C12B—C13B—H13B	120.6
C5A—C6A—N2A	132.0 (3)	C11A—C12A—H12A	119.4
C5A—C6A—C1A	123.9 (3)	C13A—C12A—C11A	121.1 (3)

O1B—C10B—C9B	119.9 (3)	C13A—C12A—H12A	119.4
O1B—C10B—C11B	121.4 (3)	C16B—C15B—H15B	120.4
C9B—C10B—C11B	118.7 (3)	C14B—C15B—C16B	119.1 (3)
C6A—C1A—N1A	111.6 (3)	C14B—C15B—H15B	120.4
C2A—C1A—N1A	129.8 (3)	C13A—C14A—C11A	118.6 (3)
C2A—C1A—C6A	118.6 (3)	C15A—C14A—C11A	120.1 (3)
C16B—C11B—C10B	118.8 (3)	C15A—C14A—C13A	121.3 (3)
C12B—C11B—C10B	122.2 (3)	C12A—C13A—H13A	120.5
C12B—C11B—C16B	119.0 (3)	C14A—C13A—C12A	119.0 (3)
C6B—C5B—H5B	121.9	C14A—C13A—H13A	120.5
C6B—C5B—C4B	116.2 (3)	C16A—C15A—H15A	120.4
C4B—C5B—H5B	121.9	C14A—C15A—C16A	119.1 (3)
C16A—C11A—C10A	119.3 (3)	C14A—C15A—H15A	120.4
S1B—C9B—C10B—O1B	−15.4 (5)	C9B—C10B—C11B—C16B	143.2 (3)
S1B—C9B—C10B—C11B	165.7 (2)	C9B—C10B—C11B—C12B	−38.8 (5)
S1A—C9A—C10A—O1A	22.5 (4)	C1B—N1B—C7B—S1B	179.7 (3)
S1A—C9A—C10A—C11A	−157.4 (2)	C1B—N1B—C7B—N2B	−0.9 (3)
C11B—C14B—C13B—C12B	−179.4 (3)	C1B—C6B—C5B—C4B	−0.4 (5)
C11B—C14B—C15B—C16B	−179.9 (3)	C9A—S1A—C7A—N2A	1.5 (2)
C11A—C14A—C13A—C12A	−179.1 (3)	C9A—S1A—C7A—N1A	−179.6 (3)
C11A—C14A—C15A—C16A	178.5 (3)	C6B—N2B—C7B—S1B	−179.2 (2)
N2B—C8B—C9B—S1B	−0.5 (3)	C6B—N2B—C7B—N1B	1.2 (4)
N2B—C8B—C9B—C10B	−172.8 (3)	C6B—N2B—C8B—C9B	179.8 (3)
N2B—C6B—C5B—C4B	−180.0 (3)	C6B—C1B—C2B—C3B	0.7 (5)
N2A—C8A—C9A—S1A	0.5 (3)	C6B—C5B—C4B—C3B	0.9 (5)
N2A—C8A—C9A—C10A	172.1 (3)	C5A—C6A—C1A—N1A	178.3 (3)
N2A—C6A—C1A—N1A	0.0 (3)	C5A—C6A—C1A—C2A	−0.1 (5)
N2A—C6A—C1A—C2A	−178.3 (3)	C5A—C4A—C3A—C2A	1.1 (5)
N1B—C1B—C6B—N2B	0.4 (3)	C6A—N2A—C7A—S1A	178.3 (2)
N1B—C1B—C6B—C5B	−179.2 (3)	C6A—N2A—C7A—N1A	−0.9 (4)
N1B—C1B—C2B—C3B	179.2 (3)	C6A—N2A—C8A—C9A	−179.1 (3)
O1B—C10B—C11B—C16B	−35.7 (5)	C6A—C5A—C4A—C3A	−1.2 (5)
O1B—C10B—C11B—C12B	142.3 (4)	C6A—C1A—C2A—C3A	−0.1 (5)
N1A—C1A—C2A—C3A	−178.2 (3)	C10B—C11B—C16B—C15B	179.4 (3)
C7A—S1A—C9A—C8A	−1.1 (3)	C10B—C11B—C12B—C13B	−178.5 (3)
C7A—S1A—C9A—C10A	−173.4 (3)	C1A—N1A—C7A—S1A	−178.0 (3)
C7A—N2A—C8A—C9A	0.7 (4)	C1A—N1A—C7A—N2A	0.9 (3)
C7A—N2A—C6A—C5A	−177.5 (3)	C1A—C2A—C3A—C4A	−0.4 (5)
C7A—N2A—C6A—C1A	0.5 (3)	C11B—C16B—C15B—C14B	−1.3 (5)
C7A—N1A—C1A—C6A	−0.6 (3)	C11B—C12B—C13B—C14B	−0.2 (5)
C7A—N1A—C1A—C2A	177.6 (3)	C11A—C16A—C15A—C14A	1.5 (5)
C7B—S1B—C9B—C8B	0.8 (3)	C11A—C12A—C13A—C14A	−0.5 (5)
C7B—S1B—C9B—C10B	173.7 (3)	C2B—C1B—C6B—N2B	179.2 (3)
C7B—N2B—C8B—C9B	−0.2 (4)	C2B—C1B—C6B—C5B	−0.4 (5)
C7B—N2B—C6B—C1B	−0.9 (3)	C2B—C3B—C4B—C5B	−0.7 (5)
C7B—N2B—C6B—C5B	178.7 (3)	C10A—C11A—C16A—C15A	−177.3 (3)
C7B—N1B—C1B—C6B	0.3 (3)	C10A—C11A—C12A—C13A	176.6 (3)

C7B—N1B—C1B—C2B	−178.4 (3)	C4B—C3B—C2B—C1B	−0.1 (5)
C8B—N2B—C7B—S1B	0.8 (3)	C4A—C5A—C6A—N2A	178.5 (3)
C8B—N2B—C7B—N1B	−178.8 (3)	C4A—C5A—C6A—C1A	0.8 (5)
C8B—N2B—C6B—C1B	179.0 (3)	C16A—C11A—C10A—O1A	26.5 (5)
C8B—N2B—C6B—C5B	−1.3 (6)	C16A—C11A—C10A—C9A	−153.6 (3)
C8B—C9B—C10B—O1B	156.5 (3)	C16A—C11A—C12A—C13A	0.8 (5)
C8B—C9B—C10B—C11B	−22.5 (5)	C16B—C11B—C12B—C13B	−0.5 (5)
C8A—N2A—C7A—S1A	−1.5 (3)	C12B—C11B—C16B—C15B	1.3 (5)
C8A—N2A—C7A—N1A	179.3 (3)	C13B—C14B—C15B—C16B	0.6 (5)
C8A—N2A—C6A—C5A	2.2 (6)	C12A—C11A—C10A—O1A	−149.3 (3)
C8A—N2A—C6A—C1A	−179.8 (3)	C12A—C11A—C10A—C9A	30.6 (5)
C8A—C9A—C10A—O1A	−148.5 (3)	C12A—C11A—C16A—C15A	−1.4 (5)
C8A—C9A—C10A—C11A	31.6 (5)	C15B—C14B—C13B—C12B	0.2 (5)
C9B—S1B—C7B—N2B	−0.9 (2)	C13A—C14A—C15A—C16A	−1.1 (6)
C9B—S1B—C7B—N1B	178.6 (3)	C15A—C14A—C13A—C12A	0.6 (5)

Hydrogen-bond geometry ($\text{\AA}$, $^\circ$)

*Cg*1, and *Cg*7 are the centroids of of atoms S1A/C7A/N2A/C8A/C9A and C1B—C6B, respectively.

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
C8A—H8A $\cdots$ N1A ⁱ	0.93	2.30	3.206 (3)	165
C8B—H8B $\cdots$ N1B ⁱⁱ	0.93	2.31	3.212 (3)	163
C13B—H13B $\cdots$ <i>Cg</i> 1 ⁱⁱ	0.93	2.88	3.551 (4)	130
C16A—H16A $\cdots$ <i>Cg</i> 7 ⁱⁱⁱ	0.93	3.00	3.832 (4)	150

Symmetry codes: (i) $x, -y+1/2, z-1/2$; (ii) $x, -y+3/2, z-1/2$; (iii) $-x+1, y-1/2, -z+3/2$.