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Consistent supramolecular motifs and different local symmetries in the structures of 2-amino-5-(4-fluorophenyl)-1,3-thiazole-4-carbaldehyde and 2-amino-5-(4-chlorophenyl)-1,3-thiazole-4-carbaldehyde

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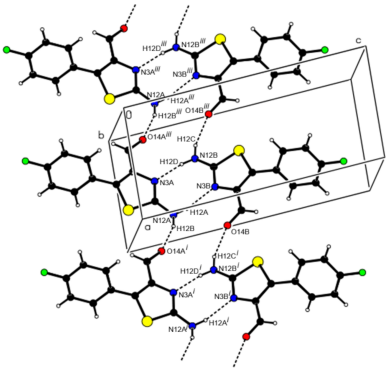
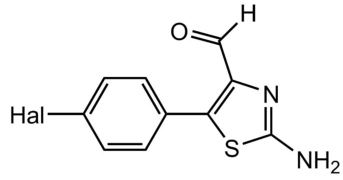
The first title compound, $C_{10}H_7FN_2OS$, crystallizes in space group $P\overline{1}$ with two independent molecules in the asymmetric unit, which form a dimer with an $R_2^2(8)$ motif through pairwise N—H···N hydrogen bonds. In the crystal of (I), N—H···O hydrogen bonds bind the dimers into zigzag ribbons running along the [100] direction, generating $R_4^4(14)$ motifs. The second title compound, $C_{10}H_7ClN_2OS$ (space group $I2/a$), contains one molecule in the asymmetric unit, which forms a dimer with an $R_2^2(8)$ motif *via* inversion symmetry. In the extended structure, the molecules form zigzag ribbons in the [100] direction by N—H···N and N—H···O hydrogen bonds, resulting in consecutive $R_1^4(8)R_1^2(5)R_2^2(8)R_1^2(5)R_1^4(8)$ motifs. The Hirshfeld surface analyses of the compounds (I) and (II) indicates that the most important factors influencing the crystal packing are H···H interactions [21.1% for molecule *A* of (I), 20.3% for molecule *B* of (I) and 21.0% for (II)].

1. Chemical context

Thiazole and its derivatives are known for their broad spectrum of biological applications, such as antimicrobial, anti-inflammatory, antiviral, antitubercular and CNS active agents and for their anticancer activities (Basarab *et al.*, 2012; Shaikh *et al.*, 2023). It should be noted that the thiazole-4-carbaldehyde fragment is part of the natural polyketide thuggacin A, which has high anti-tuberculosis activity (Liu *et al.*, 2025). Earlier, we showed that acetal-containing chlorooxiranes and their isomeric chloroketones are effective starting reagents for obtaining heterocyclic systems, in particular, heterocyclic aldehydes (Guseinov & Yudina, 1998; Guseinov *et al.*, 2017).





Hal = F (**I**), Cl (**II**)

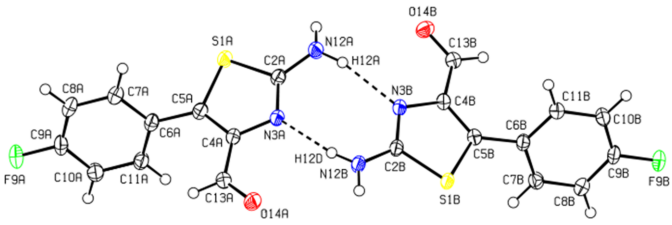


Figure 1
The asymmetric unit of (I) with displacement ellipsoids drawn at the 50% probability level.

In this work, we describe a one-step synthetic protocol to access 2-amino-5-(4-halophenyl)thiazole-4-carbaldehydes and a study of their structural features using X-ray diffraction.

2. Structural commentary

Compound (I) crystallizes in the triclinic space group $P\overline{1}$ with two crystallographically independent molecules, *A* and *B*, in the asymmetric unit (Fig. 1). An overlay fit of inverted molecule *B* on molecule *A* is shown in supplementary Fig. S1: the weighted r.m.s. fit of the 15 non-H atoms being 0.114 Å with the major differences being in the terminal benzene rings of molecules *A* and *B*. The dihedral angle between the planes of the five and six-membered rings is 61.74 (8)° for *A* and 57.07 (8)° for *B*. Selected bond lengths include C9*A*—F9*A* = 1.3580 (18) Å for molecule *A* and C9*B*—F9*B* = 1.3626 (17) Å for molecule B. The C—N bond lengths in the five-membered rings are C2*A*—N3*A* = 1.308 (2) and C4*A*—N3*A* = 1.384 (2) Å for *A* and C2*B*—N3*B* = 1.309 (2) and C4*B*—N3*B* = 1.388 (2) Å for *B*. The C—N bond length attached to the five-membered ring of the NH_2 group is C2*A*—N12*A* = 1.343 (2) Å for *A* and C2*B*—N12*B* = 1.344 (2) Å for *B*.

Compound (II), which crystallizes in space group *I*2/*a* with one molecule in the asymmetric unit (Fig. 2) has a non planar conformation in which the dihedral angle between the planes of the benzene and 1,3-thiazole rings is 56.50 (8)°. The torsion angles S1—C5—C6—C7 and C4—C5—C6—C11 are −57.7 (2) and −53.7 (3)°, respectively. The C—N lengths [C2—N3 and C4—N3] in the five-membered ring are 1.307 (2) and 1.386 (2) Å, respectively. The C—N length [C2—N12] for the NH_2 group attached to the ring is 1.346 (2) Å and the C9—Cl9 bond length is 1.7410 (16) Å.

Otherwise, the bond lengths and angles in compounds (I) and (II) are normal and can be compared with each other and with those in the *Database Survey* section.

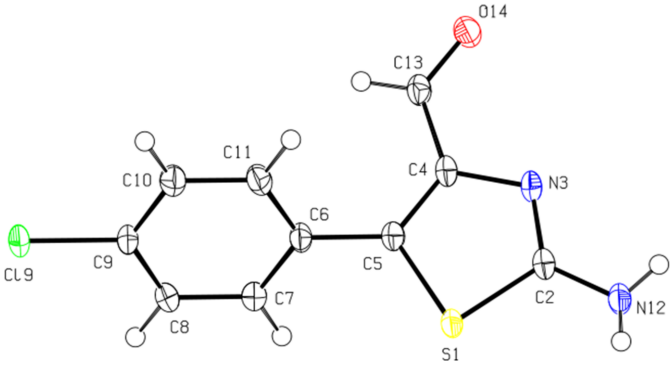


Figure 2
The asymmetric unit of (II) with displacement ellipsoids drawn at the 50% probability level.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N12*A*—H12*A*···N3*B*	0.87 (2)	2.16 (3)	3.0121 (19)	167 (2)
N12*A*—H12*B*···O14*A*^{i}	0.86 (2)	2.13 (2)	2.9596 (19)	160 (2)
N12*B*—H12*C*···O14*B*^{ii}	0.82 (2)	2.16 (2)	2.9433 (19)	161 (2)
N12*B*—H12*D*···N3*A*	0.87 (3)	2.13 (3)	2.9778 (19)	164 (2)
C8*A*—H8*A*···S1*B*^{iii}	0.95	2.91	3.6376 (16)	134
C8*B*—H8*B*···N3*A*^{iv}	0.95	2.68	3.521 (2)	149
C13*B*—H13*B*···F9*A*^{v}	0.95	2.60	3.4911 (19)	157
C7*B*—H7*B*···*Cg*3^{iv}	0.95	2.75	3.4117 (17)	127

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N12—H12*A*···N3^{i}	0.84 (3)	2.19 (3)	3.015 (2)	167 (2)
N12—H12*A*···O14^{i}	0.84 (3)	2.61 (3)	3.1222 (19)	121 (2)
N12—H12*B*···O14^{ii}	0.81 (3)	2.18 (3)	2.940 (2)	159 (2)
C9—Cl9···*Cg*1^{iii}	1.74 (1)	3.53 (1)	4.5317 (19)	114 (1)

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

3. Supramolecular features and Hirshfeld surface analyses

The two independent molecules (*A* and *B*) in the asymmetric unit of (I) form a dimer with an $R_2^2(8)$ motif through pairwise N—H···N hydrogen bonds (Table 1). In the crystal,

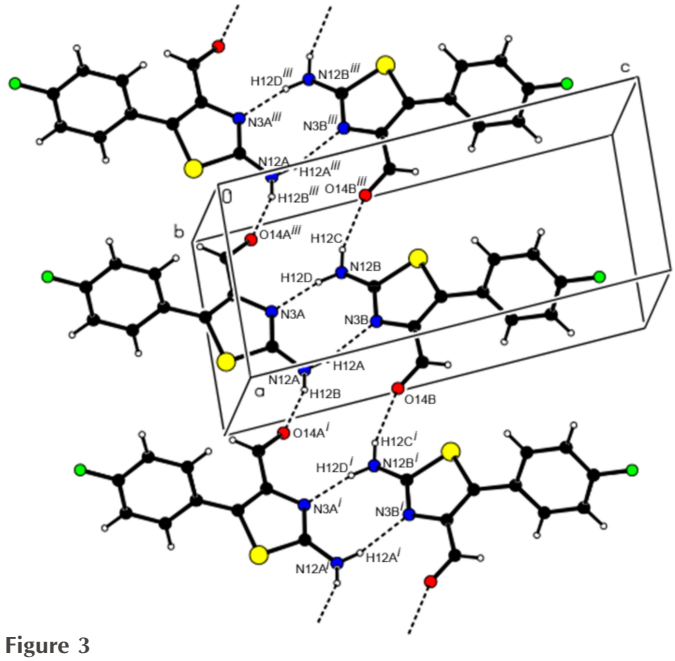


Figure 3
Partial packing diagram for (I) showing ribbons extending along the [100] direction with an $[R_2^2(8)R_4^4(14)]_n$ motif formed by N—H···N and N—H···O hydrogen bonds. Symmetry codes: (i) $x+1, y, z$; (iii) $x-1, y, z$.

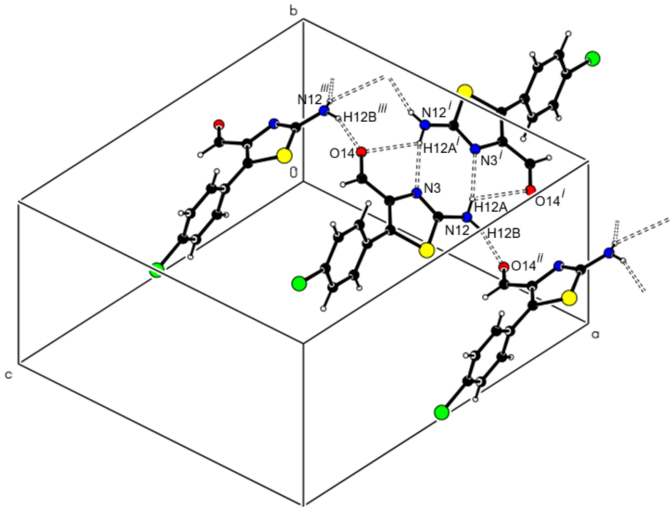


Figure 4
A partial view of the packing of (II) showing N—H···N and N—H···O hydrogen bonds, forming zigzag ribbons propagating along the [100] direction, with successive $[R_1^4(8)R_1^2(5)R_2^2(8)R_1^2(5)R_1^4(8)]_n$ motifs. Symmetry codes: (i) $-x+1, -y+1, -z$; (ii) $x+\frac{1}{2}, -y+1, z$; (iii) $x+\frac{1}{2}, -y+1, z$.

N—H···O hydrogen bonds link the dimers into zigzag ribbons extending along the [100] direction, producing $R_4^4(14)$ motifs between them (Fig. 3). Additionally, the molecules in these ribbons form $R_2^3(11)$ motifs through C—H···S and C—H···F interactions, resulting in a three-dimensional supramolecular network. A weak C—H···π interaction also occurs (supplementary Figs. S2–S4).

In the extended structure of (II), the molecules are linked through N—H···N and N—H···O hydrogen bonds (Table 2), forming zigzag ribbons propagating along the [100] direction, generating successive $R_1^4(8)R_1^2(5)R_2^2(8)R_1^2(5)R_1^4(8)$ motifs (Fig. 4). In addition, π–π [$Cg2\cdots Cg2^a$ = 3.8099 (11) Å, slippage = 1.011 Å; symmetry code (*a*) $\frac{3}{2}-x, y, 1-z$; *Cg*2 is the centroid of the (C6–C11) benzene ring] and C—Cl···π interactions (Table 1) connect these ribbons along the [010] and [001] directions to generate a three-dimensional supramolecular network (supplementary Figs. S5–S7).

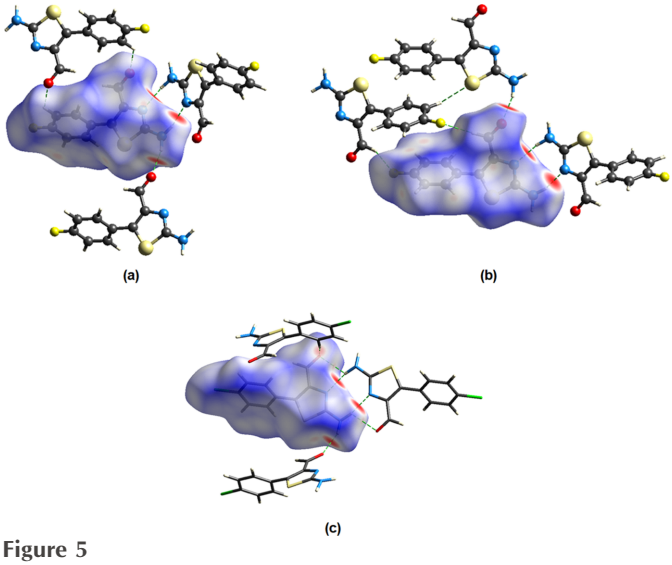


Figure 5
View of the three-dimensional Hirshfeld surfaces of the molecules *A* (*a*) and *B* (*b*) of (I), and (*c*) (II) plotted over d_{norm}.

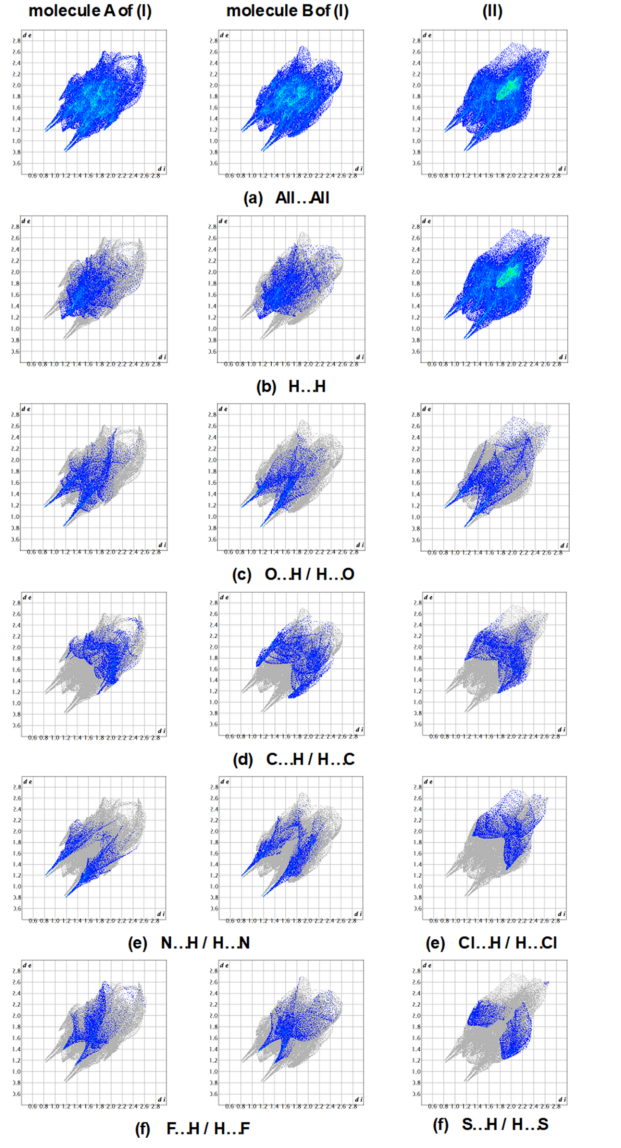


Figure 6
Two-dimensional fingerprint plots of molecules *A* and *B* of (I), and (II) showing (*a*) all interactions, and delineated into (*b*) H···H, (*c*) O···H/H···O, (*d*) C···H/H···C, (*e*) N···H/H···N for *A* and *B* of (I) and Cl···H/H···Cl for (II), and (*f*) F···H/H···F for *A* and *B* of (I) and S···H/H···S for (II), interactions.

Crystal Explorer 21 (Spackman *et al.*, 2021) was used to construct Hirshfeld surfaces for both independent molecules *A* and *B* in the asymmetric unit of compound (I). The d_{norm} mappings for molecule *A* were performed in the range of −0.49 to +1.11 a.u., and for molecule *B* in the range of −0.49 to +1.11 a.u. On the d_{norm} surfaces, bold red circles show the locations of N—H···O and N—H···N interactions (Fig. 5). Smaller red spots are caused by the C—H···S interactions.

Fingerprint plots (Fig. 6) for (I) reveal that H···H (21.1% for molecule *A* and 20.3% for molecule *B*) interactions make the largest contributions to the surface contacts and O···H/H···O (16.0% for *A* and 13.5% for *B*), C···H/H···C (13.1%

for *A* and 16.1% for *B*), N···H/H···N (11.7% for *A* and 13.1% for *B*) and F···H/H···F (10.3% for *A* and 10.2% for *B*) contacts are also significant. The interactions that have less of an influence include S···H/H···S (9.7% for *A* and 6.2% for *B*), C···C (5.6% for *A* and 5.8% for *B*), F···C/C···F (4.3% for *A* and *B*), S···F/F···S (2.6% for *A* and 3.2% for *B*), S···C/C···S (1.9% for *A* and 2.7% for *B*), F···O/O···F (1.0% for *A* and 0.9% for *B*), F···F (0.6% for *A* and 0.0% for *B*) and F···N/N···F (0.2% for *A* and *B*).

The solid-state consolidation in (II) is significantly impacted by H···H interactions, which account for 21.0% of the total. The interactions that have less of an influence include O···H/H···O (15.3%), C···H/H···C (12.1%), Cl···H/H···Cl (9.9%) and S···H/H···S (7.9%), C···C (6.8%), Cl···C/C···Cl (6.7%), Cl···S/S···Cl (3.7%), S···O / O···S (2.1%), Cl···Cl (1.8%), Cl···N/N···Cl (0.8%), N···C/C···N (0.5%), S···S (0.31%) and S···C / C···S (0.2%).

While the contributions of the strong interactions of (I) and (II) are quite consistent, weak interactions vary slightly depending on the molecular conformation and the environment of the molecules.

4. Database survey

The most closely related ten structures containing a 5-phenyl-1,3-thiazole fragment are as follows: Cambridge Structural Database (CSD, Version 6.00, update of April 2025; Groom *et al.*, 2016) refcodes MEFVUS (Guseinov *et al.*, 2022), IQUHOT (Saravanan *et al.*, 2016), GUVVAW (Akkurt *et al.*, 2015), WOJKOX (Mague *et al.*, 2014), HOQSAJ (El Ashry *et al.*, 2014), SAYXEW (Sun *et al.*, 2006), EKEZUP (Rybakov *et al.*, 2003), HIYLOQ (Au-Alvarez *et al.*, 1999), FUHJIB (Caldwell *et al.*, 1987) and CPYPTZ (Le Count & Jarvis, 1977).

In the crystal of MEFVUS, C—H···π interactions link the molecules, forming a three-dimensional network. In IQUHOT, the molecules are linked *via* C—H···O interactions, which form *C*(7) chains propagating along [010]. In the crystal of GUVVAW, the molecular packing features C—H···O and C—H···π interactions, forming a three-dimensional network. In WOJKOX, the two independent molecules are associated *via* complementary N—H···N hydrogen bonds into a dimer. These dimers are associated through weak C— H···Cl and C—H···S interactions into supramolecular chains propagating along the *a*-axis direction. In HOQSAJ, molecular pairs connect by forming $R_2^2(8)$ motifs *via* N—H···N interactions. A three-dimensional network is established through C—H···π and C—Br···π interactions. In SAYXEW, similarly to HOQSAJ, molecular pairs come together *via* N—H···N interactions to form $R_2^2(8)$ motifs. A three-dimensional network is formed with C—H···π interactions. In EKEZUP, molecules form extended chains through O—H···N hydrogen bonds. In HIYLOQ, molecules are linked in parallel layers through N—H···N and N—H···S interactions in the *bc* plane. The layers are connected by C—H···π interactions. In FUHJIB, molecules are connected to each other by forming ribbons in the [110] direction. The molecular packing features C—H···O and C—H···F interactions. Additional C—F···π and C—O···π interactions consolidate the packing. In CPYPTZ, molecules are linked in the *b*-axis direction as *C*(7) zigzag chains through N—H···N interactions. The molecules form a three-dimensional network *via* C≡C···π interactions.

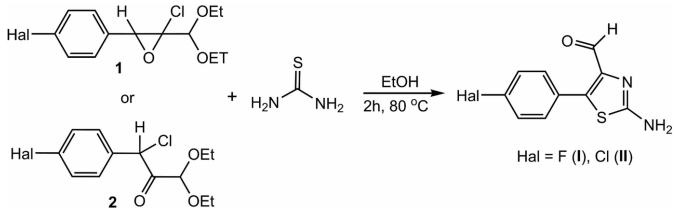


Figure 7
Synthesis scheme for (I) and (II).

5. Synthesis and crystallization

To a solution of 2-chloro-2-(diethoxymethyl)-3-(4-fluorophenyl)oxirane [also called 1-chloro-3,3-diethoxy-1-(4-fluorophenyl)propan-2-one] (1.00 mmol) in 20 ml of ethanol (95%) was added thiourea (1.00 mmol) and refluxed at 353 K for 2 h (Fig. 7). Then the ethanol was evacuated under vacuum and the resulting yellow powder of (I) was recrystallized from diethyl ether solution. Crystals suitable for X-ray diffraction were obtained by crystallization of this yellow powder from dimethylsulfoxide (DMSO) solution: yield: 91 or 73%; m.p. 378–380 K. Analysis calculated (%) for $C_{10}H_7FN_2OS$: C 54.05, H 3.17, N 12.61; found C 54.04, H 3.15, N 12.58. ^{1}H NMR (300MHz, DMSO-d_6): 6.73 (2H, NH2), 7.38–7.75 (4H, Ar), 9.48 (1H, CHO). ^{13}C NMR (75MHz, DMSO-d_6): 116.07, 116.51, 124.00, 132.13, 132.30, 136.44, 137.62, 160.66, 165.60, 167.03, 180.12.

2-Chloro-2-(diethoxymethyl)-3-(4-chlorophenyl)oxirane [also called 1-chloro-3,3-diethoxy-1-(4-chlorophenyl)propan-2-one] was used as a starting material in the synthesis of (II), otherwise the synthetic procedure was the same as for (I): yield: 95 or 77%; m.p. 397–398 K. Analysis calculated (%) for $C_{10}H_7ClN_2OS$: C 50.32, H 2.96, N 11.74; found C 50.28 H 2.95, N 11.70. ^{1}H NMR (300MHz, DMSO-d_6): 7.51–7.66 (4H, Ar), 8.36 (2H, NH2), 9.48 (1H, CHO). ^{13}C NMR (75MHz, DMSO-d_6): 126.18, 129.42, 131.67, 135.08, 135.49, 136.94, 167.45, 179.75.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The C-bound H atoms were positioned geometrically and refined using a riding model, with C—H = 0.95 Å. The H atoms of the NH_2 groups were found in difference-Fourier maps and their positions were freely refined.

Acknowledgements

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Table 3
Experimental details.

	(I)	(II)
Crystal data		
Chemical formula	$C_{10}H_7FN_2OS$	$C_{10}H_7ClN_2OS$
M_r	222.24	238.69
Crystal system, space group	Triclinic, $P\overline{1}$	Monoclinic, $I2/a$
Temperature (K)	100	100
a, b, c (Å)	7.6272 (1), 9.0292 (1), 14.7403 (3)	13.9857 (2), 9.8459 (1), 15.3349 (2)
α, β, γ (°)	90.567 (1), 98.122 (1), 108.526 (1)	90, 105.170 (1), 90
V (Å^3)	951.24 (3)	2038.06 (5)
Z	4	8
Radiation type	Cu $K\alpha$	Cu $K\alpha$
μ (mm^{-1})	2.95	5.01
Crystal size (mm)	0.27 × 0.22 × 0.15	0.53 × 0.38 × 0.30
Data collection		
Diffractometer	XtaLAB Synergy, Dualflex, HyPix	XtaLAB Synergy, Dualflex, HyPix
Absorption correction	Gaussian (*CrysAlis PRO*; Rigaku OD, 2025)	Gaussian (CrysAlisPr; (Rigaku OD, 2025)
T_{min}, T_{max}	0.482, 0.642	0.169, 0.859
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	25299, 4097, 3888	13963, 2220, 2165
R_{int}	0.047	0.043
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.638	0.639
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.036, 0.098, 1.09	0.036, 0.094, 1.07
No. of reflections	4097	2220
No. of parameters	287	144
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.30, −0.32	0.37, −0.37

Computer programs: *CrysAlis PRO* (Rigaku OD, 2025), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2020).

Russian State Agrarian University–Moscow Timiryazev Agricultural Academy, Erciyes University (Türkiye), Baku State University (Azerbaijan), and Azerbaijan Medical University. The authors' contributions are as follows. Conceptualization, FIG, MA, and ANB; synthesis, KAA and SMG; X-ray analysis, AMP and FSA; writing (review and editing of the manuscript), FIG, KIH, and MA; funding acquisition, FSA and KIH; supervision, FIG, MA, and ANB.

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supporting information

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Consistent supramolecular motifs and different local symmetries in the structures of 2-amino-5-(4-fluorophenyl)-1,3-thiazole-4-carbaldehyde and 2-amino-5-(4-chlorophenyl)-1,3-thiazole-4-carbaldehyde

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Computing details

2-Amino-5-(4-fluorophenyl)-1,3-thiazole-4-carbaldehyde (I)

Crystal data

$C_{10}H_7FN_2OS$
$M_r = 222.24$
Triclinic, $P\overline{1}$
$a = 7.6272$ (1) Å
$b = 9.0292$ (1) Å
$c = 14.7403$ (3) Å
$\alpha = 90.567$ (1)°
$\beta = 98.122$ (1)°
$\gamma = 108.526$ (1)°
$V = 951.24$ (3) Å^3
$Z = 4$
$F(000) = 456$
$D_x = 1.552$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 15352 reflections
$\theta = 3.0$–$79.1°$
$\mu = 2.95$ mm^{-1}
$T = 100$ K
Prism, yellow
0.27 × 0.22 × 0.15 mm

Data collection

XtaLAB Synergy, Dualflex, HyPix diffractometer
Radiation source: micro-focus sealed X-ray tube, PhotonJet (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: gaussian (CrysAlisPro; Rigaku OD, 2025)
$T_{min} = 0.482$, $T_{max} = 0.642$
25299 measured reflections
4097 independent reflections
3888 reflections with $I > 2\sigma(I)$
$R_{int} = 0.047$
$\theta_{max} = 79.8°$, $\theta_{min} = 3.0°$
$h = -9 \rightarrow 9$
$k = -11 \rightarrow 11$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.098$
$S = 1.09$
4097 reflections
287 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0488P)^2 + 0.4701P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ 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}
C2A	0.6615 (2)	0.83196 (18)	0.12921 (10)	0.0221 (3)
C2B	0.4924 (2)	0.83630 (18)	0.38518 (10)	0.0213 (3)
C4A	0.3723 (2)	0.77903 (18)	0.05708 (10)	0.0220 (3)
C4B	0.7501 (2)	0.80308 (18)	0.45848 (10)	0.0219 (3)
C5A	0.4497 (2)	0.75647 (19)	−0.01828 (11)	0.0229 (3)
C5B	0.6445 (2)	0.76230 (18)	0.52804 (10)	0.0215 (3)
C6A	0.3598 (2)	0.70487 (19)	−0.11352 (10)	0.0232 (3)
C6B	0.6890 (2)	0.71135 (18)	0.62088 (10)	0.0214 (3)
C7A	0.4107 (2)	0.80140 (19)	−0.18549 (11)	0.0257 (3)
H7A	0.507656	0.899145	−0.173195	0.031*
C7B	0.5773 (2)	0.56850 (19)	0.64774 (11)	0.0238 (3)
H7B	0.474834	0.504211	0.605476	0.029*
C8A	0.3209 (2)	0.7556 (2)	−0.27469 (11)	0.0274 (3)
H8A	0.352042	0.822314	−0.323469	0.033*
C8B	0.6136 (2)	0.51914 (19)	0.73517 (11)	0.0245 (3)
H8B	0.538805	0.421354	0.753172	0.029*
C9A	0.1857 (2)	0.6112 (2)	−0.29078 (11)	0.0271 (3)
C9B	0.7615 (2)	0.6165 (2)	0.79501 (10)	0.0236 (3)
C10A	0.1335 (2)	0.5107 (2)	−0.22235 (12)	0.0276 (3)
H10A	0.040183	0.411258	−0.235969	0.033*
C10B	0.8742 (2)	0.7586 (2)	0.77200 (11)	0.0261 (3)
H10B	0.974704	0.822805	0.815248	0.031*
C11A	0.2213 (2)	0.5591 (2)	−0.13282 (11)	0.0252 (3)
H11A	0.186923	0.492471	−0.084345	0.030*
C11B	0.8374 (2)	0.80602 (19)	0.68379 (11)	0.0241 (3)
H11B	0.913848	0.903551	0.666320	0.029*
C13A	0.1778 (2)	0.7715 (2)	0.05284 (11)	0.0256 (3)
H13A	0.097536	0.741770	−0.004340	0.031*
C13B	0.9386 (2)	0.79426 (19)	0.46269 (11)	0.0244 (3)
H13B	0.993238	0.760225	0.517060	0.029*
F9A	0.09835 (16)	0.56466 (13)	−0.37805 (7)	0.0361 (3)
F9B	0.79817 (14)	0.56898 (12)	0.88103 (6)	0.0293 (2)
N3A	0.49060 (18)	0.82060 (15)	0.14004 (9)	0.0215 (3)
N3B	0.66485 (18)	0.84586 (16)	0.37814 (9)	0.0216 (3)
N12A	0.8086 (2)	0.87201 (17)	0.19689 (10)	0.0257 (3)
N12B	0.3726 (2)	0.86969 (18)	0.31901 (9)	0.0247 (3)
O14A	0.11253 (16)	0.80146 (16)	0.11929 (8)	0.0305 (3)
O14B	1.02965 (16)	0.82851 (15)	0.39967 (8)	0.0294 (3)
S1A	0.68838 (5)	0.79416 (5)	0.01534 (3)	0.02509 (11)

S1B	0.42376 (5)	0.77503 (5)	0.49132 (2)	0.02230 (11)
H12A	0.786 (3)	0.873 (3)	0.2530 (17)	0.036 (6)*
H12B	0.911 (3)	0.856 (2)	0.1879 (15)	0.029 (5)*
H12C	0.265 (3)	0.853 (2)	0.3284 (15)	0.028 (5)*
H12D	0.392 (3)	0.865 (3)	0.2623 (19)	0.043 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C2A	0.0243 (7)	0.0251 (7)	0.0184 (7)	0.0090 (6)	0.0054 (6)	0.0024 (6)
C2B	0.0240 (7)	0.0248 (7)	0.0153 (7)	0.0081 (6)	0.0033 (5)	0.0016 (5)
C4A	0.0232 (7)	0.0257 (7)	0.0172 (7)	0.0078 (6)	0.0038 (6)	0.0026 (6)
C4B	0.0229 (7)	0.0248 (7)	0.0166 (7)	0.0064 (6)	0.0013 (6)	0.0018 (5)
C5A	0.0251 (7)	0.0254 (7)	0.0198 (7)	0.0094 (6)	0.0055 (6)	0.0040 (6)
C5B	0.0216 (7)	0.0242 (7)	0.0176 (7)	0.0066 (6)	0.0011 (6)	0.0000 (6)
C6A	0.0270 (7)	0.0293 (8)	0.0171 (7)	0.0137 (6)	0.0054 (6)	0.0032 (6)
C6B	0.0231 (7)	0.0272 (8)	0.0155 (7)	0.0107 (6)	0.0028 (5)	0.0017 (6)
C7A	0.0311 (8)	0.0274 (8)	0.0207 (8)	0.0110 (6)	0.0072 (6)	0.0020 (6)
C7B	0.0248 (7)	0.0266 (8)	0.0194 (7)	0.0084 (6)	0.0012 (6)	−0.0020 (6)
C8A	0.0363 (9)	0.0327 (8)	0.0183 (7)	0.0159 (7)	0.0092 (6)	0.0065 (6)
C8B	0.0288 (8)	0.0253 (7)	0.0205 (7)	0.0094 (6)	0.0058 (6)	0.0041 (6)
C9A	0.0321 (8)	0.0370 (9)	0.0157 (7)	0.0175 (7)	0.0007 (6)	−0.0003 (6)
C9B	0.0291 (8)	0.0319 (8)	0.0136 (7)	0.0153 (6)	0.0034 (6)	0.0037 (6)
C10A	0.0285 (8)	0.0303 (8)	0.0235 (8)	0.0099 (7)	0.0019 (6)	0.0014 (6)
C10B	0.0259 (8)	0.0323 (8)	0.0190 (7)	0.0095 (6)	−0.0011 (6)	0.0000 (6)
C11A	0.0277 (8)	0.0298 (8)	0.0197 (7)	0.0110 (6)	0.0046 (6)	0.0055 (6)
C11B	0.0236 (7)	0.0273 (8)	0.0202 (7)	0.0070 (6)	0.0020 (6)	0.0031 (6)
C13A	0.0220 (7)	0.0342 (8)	0.0200 (7)	0.0083 (6)	0.0024 (6)	0.0016 (6)
C13B	0.0223 (7)	0.0284 (8)	0.0215 (7)	0.0074 (6)	0.0019 (6)	0.0033 (6)
F9A	0.0448 (6)	0.0443 (6)	0.0173 (5)	0.0153 (5)	−0.0030 (4)	−0.0012 (4)
F9B	0.0375 (5)	0.0352 (5)	0.0157 (4)	0.0133 (4)	0.0017 (4)	0.0060 (4)
N3A	0.0219 (6)	0.0266 (6)	0.0168 (6)	0.0082 (5)	0.0039 (5)	0.0024 (5)
N3B	0.0221 (6)	0.0272 (6)	0.0157 (6)	0.0082 (5)	0.0027 (5)	0.0016 (5)
N12A	0.0219 (7)	0.0369 (8)	0.0191 (7)	0.0109 (6)	0.0032 (5)	−0.0011 (5)
N12B	0.0227 (7)	0.0383 (8)	0.0167 (6)	0.0140 (6)	0.0048 (5)	0.0051 (5)
O14A	0.0261 (6)	0.0447 (7)	0.0237 (6)	0.0140 (5)	0.0077 (5)	0.0019 (5)
O14B	0.0244 (6)	0.0378 (7)	0.0282 (6)	0.0109 (5)	0.0087 (5)	0.0069 (5)
S1A	0.0238 (2)	0.0362 (2)	0.01781 (19)	0.01206 (16)	0.00570 (14)	0.00075 (15)
S1B	0.02187 (19)	0.0323 (2)	0.01454 (18)	0.01058 (15)	0.00423 (13)	0.00355 (14)

Geometric parameters (Å, º)

C2A—N3A	1.308 (2)	C7B—H7B	0.9500
C2A—N12A	1.343 (2)	C8A—C9A	1.375 (3)
C2A—S1A	1.7623 (16)	C8A—H8A	0.9500
C2B—N3B	1.309 (2)	C8B—C9B	1.377 (2)
C2B—N12B	1.344 (2)	C8B—H8B	0.9500
C2B—S1B	1.7585 (15)	C9A—F9A	1.3580 (18)

C4A—C5A	1.372 (2)	C9A—C10A	1.379 (2)
C4A—N3A	1.384 (2)	C9B—F9B	1.3626 (17)
C4A—C13A	1.455 (2)	C9B—C10B	1.375 (2)
C4B—C5B	1.374 (2)	C10A—C11A	1.391 (2)
C4B—N3B	1.388 (2)	C10A—H10A	0.9500
C4B—C13B	1.458 (2)	C10B—C11B	1.392 (2)
C5A—C6A	1.473 (2)	C10B—H10B	0.9500
C5A—S1A	1.7391 (16)	C11A—H11A	0.9500
C5B—C6B	1.477 (2)	C11B—H11B	0.9500
C5B—S1B	1.7342 (16)	C13A—O14A	1.224 (2)
C6A—C11A	1.397 (2)	C13A—H13A	0.9500
C6A—C7A	1.399 (2)	C13B—O14B	1.222 (2)
C6B—C11B	1.394 (2)	C13B—H13B	0.9500
C6B—C7B	1.398 (2)	N12A—H12A	0.87 (2)
C7A—C8A	1.387 (2)	N12A—H12B	0.86 (2)
C7A—H7A	0.9500	N12B—H12C	0.82 (2)
C7B—C8B	1.388 (2)	N12B—H12D	0.87 (3)

N3A—C2A—N12A	124.52 (14)	C7B—C8B—H8B	121.1
N3A—C2A—S1A	114.34 (12)	F9A—C9A—C8A	118.78 (15)
N12A—C2A—S1A	121.12 (12)	F9A—C9A—C10A	118.06 (16)
N3B—C2B—N12B	124.89 (14)	C8A—C9A—C10A	123.16 (15)
N3B—C2B—S1B	114.47 (11)	F9B—C9B—C10B	118.52 (14)
N12B—C2B—S1B	120.64 (12)	F9B—C9B—C8B	118.27 (14)
C5A—C4A—N3A	117.22 (14)	C10B—C9B—C8B	123.21 (14)
C5A—C4A—C13A	123.57 (14)	C9A—C10A—C11A	118.06 (16)
N3A—C4A—C13A	119.09 (13)	C9A—C10A—H10A	121.0
C5B—C4B—N3B	116.79 (14)	C11A—C10A—H10A	121.0
C5B—C4B—C13B	123.91 (14)	C9B—C10B—C11B	118.36 (15)
N3B—C4B—C13B	119.19 (13)	C9B—C10B—H10B	120.8
C4A—C5A—C6A	129.84 (15)	C11B—C10B—H10B	120.8
C4A—C5A—S1A	108.53 (12)	C10A—C11A—C6A	120.60 (15)
C6A—C5A—S1A	121.61 (12)	C10A—C11A—H11A	119.7
C4B—C5B—C6B	131.24 (14)	C6A—C11A—H11A	119.7
C4B—C5B—S1B	108.86 (11)	C10B—C11B—C6B	120.44 (15)
C6B—C5B—S1B	119.89 (11)	C10B—C11B—H11B	119.8
C11A—C6A—C7A	119.25 (15)	C6B—C11B—H11B	119.8
C11A—C6A—C5A	120.25 (14)	O14A—C13A—C4A	123.26 (15)
C7A—C6A—C5A	120.50 (15)	O14A—C13A—H13A	118.4
C11B—C6B—C7B	119.10 (14)	C4A—C13A—H13A	118.4
C11B—C6B—C5B	121.07 (14)	O14B—C13B—C4B	123.17 (15)
C7B—C6B—C5B	119.79 (14)	O14B—C13B—H13B	118.4
C8A—C7A—C6A	120.52 (16)	C4B—C13B—H13B	118.4
C8A—C7A—H7A	119.7	C2A—N3A—C4A	110.35 (13)
C6A—C7A—H7A	119.7	C2B—N3B—C4B	110.30 (13)
C8B—C7B—C6B	121.03 (15)	C2A—N12A—H12A	117.5 (16)
C8B—C7B—H7B	119.5	C2A—N12A—H12B	119.2 (14)
C6B—C7B—H7B	119.5	H12A—N12A—H12B	118 (2)

C9A—C8A—C7A	118.37 (15)	C2B—N12B—H12C	117.4 (15)
C9A—C8A—H8A	120.8	C2B—N12B—H12D	118.1 (17)
C7A—C8A—H8A	120.8	H12C—N12B—H12D	118 (2)
C9B—C8B—C7B	117.85 (15)	C5A—S1A—C2A	89.53 (7)
C9B—C8B—H8B	121.1	C5B—S1B—C2B	89.59 (7)

N3A—C4A—C5A—C6A	176.64 (15)	F9B—C9B—C10B—C11B	179.38 (14)
C13A—C4A—C5A—C6A	−7.5 (3)	C8B—C9B—C10B—C11B	−0.3 (3)
N3A—C4A—C5A—S1A	−1.54 (18)	C9A—C10A—C11A—C6A	−0.7 (2)
C13A—C4A—C5A—S1A	174.34 (13)	C7A—C6A—C11A—C10A	−0.6 (2)
N3B—C4B—C5B—C6B	179.83 (15)	C5A—C6A—C11A—C10A	178.85 (15)
C13B—C4B—C5B—C6B	3.8 (3)	C9B—C10B—C11B—C6B	0.3 (2)
N3B—C4B—C5B—S1B	0.85 (18)	C7B—C6B—C11B—C10B	0.3 (2)
C13B—C4B—C5B—S1B	−175.17 (13)	C5B—C6B—C11B—C10B	178.03 (15)
C4A—C5A—C6A—C11A	−60.0 (2)	C5A—C4A—C13A—O14A	−175.19 (17)
S1A—C5A—C6A—C11A	118.02 (15)	N3A—C4A—C13A—O14A	0.6 (3)
C4A—C5A—C6A—C7A	119.5 (2)	C5B—C4B—C13B—O14B	178.76 (16)
S1A—C5A—C6A—C7A	−62.50 (19)	N3B—C4B—C13B—O14B	2.8 (2)
C4B—C5B—C6B—C11B	58.8 (2)	N12A—C2A—N3A—C4A	179.29 (15)
S1B—C5B—C6B—C11B	−122.33 (15)	S1A—C2A—N3A—C4A	0.69 (17)
C4B—C5B—C6B—C7B	−123.49 (19)	C5A—C4A—N3A—C2A	0.6 (2)
S1B—C5B—C6B—C7B	55.40 (19)	C13A—C4A—N3A—C2A	−175.49 (14)
C11A—C6A—C7A—C8A	2.1 (2)	N12B—C2B—N3B—C4B	−179.90 (15)
C5A—C6A—C7A—C8A	−177.39 (15)	S1B—C2B—N3B—C4B	0.31 (17)
C11B—C6B—C7B—C8B	−0.9 (2)	C5B—C4B—N3B—C2B	−0.8 (2)
C5B—C6B—C7B—C8B	−178.70 (14)	C13B—C4B—N3B—C2B	175.45 (14)
C6A—C7A—C8A—C9A	−2.2 (2)	C4A—C5A—S1A—C2A	1.52 (12)
C6B—C7B—C8B—C9B	1.0 (2)	C6A—C5A—S1A—C2A	−176.85 (14)
C7A—C8A—C9A—F9A	−179.31 (15)	N3A—C2A—S1A—C5A	−1.32 (13)
C7A—C8A—C9A—C10A	0.8 (3)	N12A—C2A—S1A—C5A	−179.98 (14)
C7B—C8B—C9B—F9B	180.00 (14)	C4B—C5B—S1B—C2B	−0.53 (12)
C7B—C8B—C9B—C10B	−0.4 (2)	C6B—C5B—S1B—C2B	−179.65 (13)
F9A—C9A—C10A—C11A	−179.26 (14)	N3B—C2B—S1B—C5B	0.13 (13)
C8A—C9A—C10A—C11A	0.6 (3)	N12B—C2B—S1B—C5B	−179.67 (14)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N12*A*—H12*A*···N3*B*	0.87 (2)	2.16 (3)	3.0121 (19)	167 (2)
N12*A*—H12*B*···O14*A*^{i}	0.86 (2)	2.13 (2)	2.9596 (19)	160 (2)
N12*B*—H12*C*···O14*B*^{ii}	0.82 (2)	2.16 (2)	2.9433 (19)	161 (2)
N12*B*—H12*D*···N3*A*	0.87 (3)	2.13 (3)	2.9778 (19)	164 (2)
C8*A*—H8*A*···S1*B*^{iii}	0.95	2.91	3.6376 (16)	134
C8*B*—H8*B*···N3*A*^{iv}	0.95	2.68	3.521 (2)	149
C13*B*—H13*B*···F9*A*^{v}	0.95	2.60	3.4911 (19)	157
C7*B*—H7*B*···*Cg*3^{iv}	0.95	2.75	3.4117 (17)	127

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

2-Amino-5-(4-chlorophenyl)-1,3-thiazole-4-carbaldehyde (II)

Crystal data

$C_{10}H_7ClN_2OS$
$M_r = 238.69$
Monoclinic, $I2/a$
$a = 13.9857$ (2) Å
$b = 9.8459$ (1) Å
$c = 15.3349$ (2) Å
$\beta = 105.170$ (1)°
$V = 2038.06$ (5) Å^3
$Z = 8$
$F(000) = 976$
$D_x = 1.556$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 9428 reflections
$\theta = 5.4$–$79.9°$
$\mu = 5.01$ mm^{-1}
$T = 100$ K
Prism, yellow
0.53 × 0.38 × 0.30 mm

Data collection

XtaLAB Synergy, Dualflex, HyPix diffractometer
Radiation source: micro-focus sealed X-ray tube, PhotonJet (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: gaussian (CrysAlisPr; (Rigaku OD, 2025)
$T_{min} = 0.169$, $T_{max} = 0.859$
13963 measured reflections
2220 independent reflections
2165 reflections with $I > 2\sigma(I)$
$R_{int} = 0.043$
$\theta_{max} = 80.3°$, $\theta_{min} = 5.4°$
$h = -17\rightarrow17$
$k = -10\rightarrow12$
$l = -19\rightarrow19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.094$
$S = 1.07$
2220 reflections
144 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0543P)^2 + 2.2643P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.37$ e Å^{-3}
$\Delta\rho_{min} = -0.37$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C2	0.59720 (12)	0.44375 (16)	0.12413 (11)	0.0197 (3)
C4	0.50163 (12)	0.54350 (17)	0.19941 (10)	0.0194 (3)
C5	0.57830 (12)	0.51273 (16)	0.27300 (10)	0.0194 (3)
C6	0.59306 (12)	0.55034 (17)	0.36882 (11)	0.0202 (3)
C7	0.61451 (13)	0.45314 (18)	0.43726 (11)	0.0227 (3)
H7	0.618549	0.360040	0.422360	0.027*
C8	0.63007 (13)	0.49141 (18)	0.52726 (11)	0.0237 (3)
H8	0.643953	0.425002	0.573823	0.028*

C9	0.62502 (13)	0.62773 (18)	0.54796 (11)	0.0230 (3)
C10	0.60396 (13)	0.72642 (18)	0.48120 (12)	0.0258 (4)
H10	0.600421	0.819419	0.496565	0.031*
C11	0.58812 (13)	0.68741 (18)	0.39163 (12)	0.0242 (4)
H11	0.573797	0.754261	0.345349	0.029*
C13	0.41003 (13)	0.60683 (17)	0.20523 (11)	0.0211 (3)
H13	0.401977	0.627562	0.263401	0.025*
Cl9	0.64554 (3)	0.67747 (4)	0.66029 (3)	0.02945 (14)
N3	0.51246 (10)	0.50539 (14)	0.11549 (9)	0.0193 (3)
N12	0.62848 (12)	0.39102 (17)	0.05542 (10)	0.0240 (3)
O14	0.34230 (9)	0.63509 (13)	0.13888 (8)	0.0242 (3)
S1	0.66956 (3)	0.42813 (4)	0.23650 (2)	0.02012 (13)
H12A	0.597 (2)	0.418 (3)	0.0043 (19)	0.033 (6)*
H12B	0.687 (2)	0.376 (2)	0.0650 (17)	0.028 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C2	0.0236 (8)	0.0222 (7)	0.0133 (7)	−0.0032 (6)	0.0052 (6)	−0.0007 (6)
C4	0.0238 (8)	0.0223 (7)	0.0128 (7)	−0.0026 (6)	0.0058 (6)	−0.0007 (6)
C5	0.0224 (7)	0.0225 (7)	0.0143 (7)	0.0001 (6)	0.0065 (6)	0.0005 (6)
C6	0.0216 (7)	0.0264 (8)	0.0131 (7)	0.0009 (6)	0.0051 (6)	−0.0016 (6)
C7	0.0261 (8)	0.0248 (8)	0.0167 (8)	0.0035 (6)	0.0050 (6)	−0.0014 (6)
C8	0.0286 (8)	0.0278 (8)	0.0138 (7)	0.0052 (6)	0.0042 (6)	0.0022 (6)
C9	0.0252 (8)	0.0310 (9)	0.0123 (7)	0.0048 (6)	0.0040 (6)	−0.0034 (6)
C10	0.0333 (9)	0.0244 (8)	0.0185 (8)	0.0029 (7)	0.0048 (7)	−0.0024 (6)
C11	0.0308 (9)	0.0249 (8)	0.0157 (8)	0.0019 (6)	0.0043 (6)	0.0020 (6)
C13	0.0266 (8)	0.0226 (7)	0.0152 (7)	−0.0011 (6)	0.0075 (6)	0.0009 (6)
Cl9	0.0417 (3)	0.0328 (2)	0.0120 (2)	0.00928 (17)	0.00381 (17)	−0.00327 (14)
N3	0.0225 (6)	0.0242 (6)	0.0118 (6)	−0.0025 (5)	0.0057 (5)	−0.0015 (5)
N12	0.0228 (7)	0.0350 (8)	0.0141 (7)	0.0030 (6)	0.0047 (6)	−0.0028 (6)
O14	0.0226 (6)	0.0308 (6)	0.0186 (6)	0.0005 (5)	0.0040 (5)	0.0010 (5)
S1	0.0216 (2)	0.0264 (2)	0.0123 (2)	0.00179 (13)	0.00437 (15)	−0.00110 (13)

Geometric parameters (Å, º)

C2—N3	1.307 (2)	C8—C9	1.385 (3)
C2—N12	1.346 (2)	C8—H8	0.9500
C2—S1	1.7620 (16)	C9—C10	1.386 (3)
C4—C5	1.372 (2)	C9—Cl9	1.7410 (16)
C4—N3	1.386 (2)	C10—C11	1.387 (2)
C4—C13	1.448 (2)	C10—H10	0.9500
C5—C6	1.477 (2)	C11—H11	0.9500
C5—S1	1.7349 (16)	C13—O14	1.227 (2)
C6—C7	1.394 (2)	C13—H13	0.9500
C6—C11	1.400 (2)	N12—H12A	0.84 (3)
C7—C8	1.392 (2)	N12—H12B	0.81 (3)
C7—H7	0.9500		

N3—C2—N12	124.85 (15)	C8—C9—C10	121.58 (15)
N3—C2—S1	114.41 (12)	C8—C9—Cl9	119.62 (13)
N12—C2—S1	120.71 (13)	C10—C9—Cl9	118.80 (14)
C5—C4—N3	116.88 (15)	C9—C10—C11	119.03 (16)
C5—C4—C13	123.91 (15)	C9—C10—H10	120.5
N3—C4—C13	119.15 (14)	C11—C10—H10	120.5
C4—C5—C6	129.71 (15)	C10—C11—C6	120.57 (16)
C4—C5—S1	108.86 (12)	C10—C11—H11	119.7
C6—C5—S1	121.23 (12)	C6—C11—H11	119.7
C7—C6—C11	119.25 (15)	O14—C13—C4	123.35 (15)
C7—C6—C5	121.58 (15)	O14—C13—H13	118.3
C11—C6—C5	119.15 (15)	C4—C13—H13	118.3
C8—C7—C6	120.52 (16)	C2—N3—C4	110.36 (14)
C8—C7—H7	119.7	C2—N12—H12A	114.3 (18)
C6—C7—H7	119.7	C2—N12—H12B	116.8 (18)
C9—C8—C7	119.04 (16)	H12A—N12—H12B	119 (2)
C9—C8—H8	120.5	C5—S1—C2	89.48 (8)
C7—C8—H8	120.5		

N3—C4—C5—C6	173.71 (16)	Cl9—C9—C10—C11	179.63 (14)
C13—C4—C5—C6	−9.2 (3)	C9—C10—C11—C6	0.2 (3)
N3—C4—C5—S1	−1.08 (18)	C7—C6—C11—C10	−0.3 (3)
C13—C4—C5—S1	176.03 (13)	C5—C6—C11—C10	−178.47 (16)
C4—C5—C6—C7	128.1 (2)	C5—C4—C13—O14	179.28 (16)
S1—C5—C6—C7	−57.7 (2)	N3—C4—C13—O14	−3.7 (3)
C4—C5—C6—C11	−53.7 (3)	N12—C2—N3—C4	178.02 (16)
S1—C5—C6—C11	120.52 (16)	S1—C2—N3—C4	0.09 (18)
C11—C6—C7—C8	0.5 (3)	C5—C4—N3—C2	0.7 (2)
C5—C6—C7—C8	178.71 (16)	C13—C4—N3—C2	−176.60 (15)
C6—C7—C8—C9	−0.7 (3)	C4—C5—S1—C2	0.89 (12)
C7—C8—C9—C10	0.6 (3)	C6—C5—S1—C2	−174.43 (14)
C7—C8—C9—Cl9	−179.35 (13)	N3—C2—S1—C5	−0.59 (13)
C8—C9—C10—C11	−0.3 (3)	N12—C2—S1—C5	−178.61 (15)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N12—H12*A*···N3^{i}	0.84 (3)	2.19 (3)	3.015 (2)	167 (2)
N12—H12*A*···O14^{i}	0.84 (3)	2.61 (3)	3.1222 (19)	121 (2)
N12—H12*B*···O14^{ii}	0.81 (3)	2.18 (3)	2.940 (2)	159 (2)
C9—Cl9···*Cg*1^{iii}	1.74 (1)	3.53 (1)	4.5317 (19)	114 (1)

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