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# *N*-(6-Chloro-1-methyl-1*H*-imidazo-[4,5-*c*]pyridin-4-yl)benzenesulfonamide

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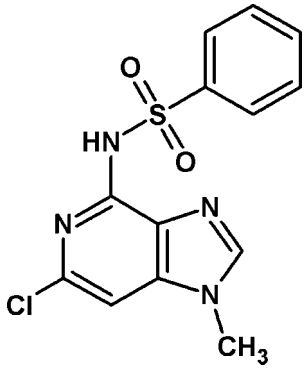
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.034; $wR$ factor = 0.098; data-to-parameter ratio = 13.1.

The asymmetric unit of the title compound, $C_{13}H_{11}ClN_4O_2S$, contains two molecules (*A* and *B*), in which the dihedral angles between the 1*H*-imidazo[4,5-*c*]pyridine system and terminal phenyl ring are 80.83 (10) and 62.34 (1)°. In the crystal, *A*–*B* dimers are linked by pairs of N—H···N hydrogen bonds, which generate $R_2^2(10)$ loops. The dimers are linked by C—H···O and C—H···Cl interactions, generating a three-dimensional network. Aromatic $\pi$–$\pi$ stacking interactions [shortest centroid–centroid distance = 3.5211 (12) Å] are also observed.

## Related literature

For biological background, see: Kulkarni & Newman (2007). For a related structure, see: Kandri Rodi *et al.* (2013).




## Experimental

### Crystal data

$C_{13}H_{11}ClN_4O_2S$
$M_r$ = 322.77
Monoclinic, $P2_1/c$
$a$ = 13.1045 (4) Å
$b$ = 14.7259 (5) Å
$c$ = 14.6953 (6) Å
$\beta$ = 95.127 (3)°
$V$ = 2824.49 (17) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.43 mm$^{-1}$
$T$ = 293 K
0.24 × 0.20 × 0.12 mm

### Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min}$ = 0.770, $T_{max}$ = 1.000
16038 measured reflections
4972 independent reflections
3759 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.031

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.098
$S$ = 1.04
4972 reflections
379 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.31 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N7*A*—H7*A*···N8*B*$^{i}$ | 0.86 | 2.25 | 3.014 (2) | 148 |
| N7*B*—H7*B*···N8*A*$^{ii}$ | 0.86 | 2.25 | 3.092 (2) | 165 |
| C13*A*—H13*A*···Cl1*A*$^{iii}$ | 0.93 | 2.82 | 3.620 (3) | 144 |
| C20*A*—H20*A*···O4*A*$^{iv}$ | 0.93 | 2.47 | 3.243 (3) | 141 |

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *SHELXL97*.

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Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7208).

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# supporting information

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## *N*-(6-Chloro-1-methyl-1*H*-imidazo[4,5-*c*]pyridin-4-yl)benzenesulfonamide

**Venkatesh B. Devaru, K. S. Katagi, O. Kotresh, H. K. Arunkashi and H. C. Devarajegowda**

### S1. Comment

Imidazo[4,5]pyridine derivatives have been reported as inhibitors of mitogen and stress-activated protein kinases and aurora kinases (Kulkarni & Newman, 2007). As part of our studies of this family of compounds, we now describe the synthesis and structure of the title compound. Its gometrical data are good agreement with those of a related structure (Kandri Rodi *et al.*, 2013)

The asymmetric unit contains two independent molecules A and B respectively are shown in Fig. 1. The 1*H*-imidazo [4,5-*c*]pyridine rings system are nearly planar, with a maximum deviations of 0.0284 (19) Å and 0.0061 (19) Å for the atoms C19*a* and C19*b*; the dihedral angles between the 1*H*-imidazo [4,5-*c*]pyridine (N5a/N6a/N8a/C15*a*–C20*a*) & (N5b/N6b/N8b/C15*b*–C20*a*) and the terminal benzene (C9a–C14*a*) & (C9b–C14*b*) rings are 80.83 (10)° and 62.34 (1)°.

In the crystal, A-B dimers are linked by pairs of N—H···N hydrogen bonds (Table 1), which generate $R^2_2(10)$ loops. The dimers are lined by C—H···O and C—H···Cl interactions to generate a three-dimensional network. Aromatic $\pi$–$\pi$ stacking interactions [shortest centroid–centroid distance = 3.5211 (12) Å] are also observed.

### S2. Experimental

A mixture of 2,4,6-trichloropyridene, methylamine in ethanol was heated and filtered to get pure product. To this sulfuric acid and fuming nitric acid was added, then it was stirred and cooled. A solution of iron powder and ammonium chloride in methanol/water was added and heated. Then triethylorthoformate in ethanol was added and continued the heating. Amination of reaction product was achieved by adding benzophenone imine, potassium carbonate, palladium complex, in dioxane, and then it was heated. The obtained product was dissolved in HCl, stirred, and concentrated *in vacuo* to give the product. A mixture of obtained product, sodium hydride, 6-chloro-1-methyl-1*H*-imidazol [4,5-*c*]pyridin-4-amine and carbonyl/sulfonyl chlorides in tetahydrofuran was stirred and concentrated *in vacuo* to give the expected products. After completion of each step of the reaction TLC was monitored. The compound is recrystallized by ethanol- chloroform mixture. Colourless needles of the title compound were grown from a mixed solution of ethanol/chloroform (v/v = 2/1) by slow evaporation at room temperature. Yield: 121 mg, 64.84%); mp: 336k; IR $cm^{-1}$ (KBr) 3435, 1388; Anal. Calcd for $C_{13}H_{11}ClN_4O_2S$ C, 45.82; H, 2.96; N, 16.44%; Found, C, 45.18; H, 2.92; N, 15.84%.

### S3. Refinement

All H atoms were positioned geometrically, with N—H = 0.86 Å, C—H = 0.93 Å for aromatic H and C—H = 0.96 Å for methyl H, and refined using a riding model with $U_{iso}$(H) = 1.5$U_{eq}$(C) for methyl H and $U_{iso}$(H) = 1.2$U_{eq}$(C) for all other H.

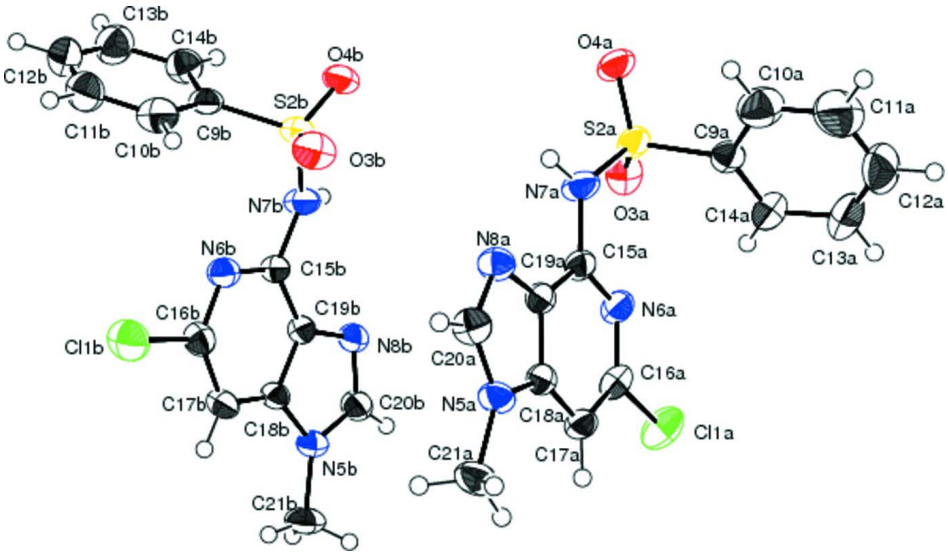


**Figure 1**

The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen bonds are shown as open dashed bonds.

### *N*-(6-Chloro-1-methyl-1*H*-imidazo[4,5-*c*]pyridin-4-yl)benzenesulfonamide

*Crystal data*

$C_{13}H_{11}ClN_4O_2S$
$M_r = 322.77$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 13.1045\ (4)$ Å
$b = 14.7259\ (5)$ Å
$c = 14.6953\ (6)$ Å
$\beta = 95.127\ (3)°$
$V = 2824.49\ (17)$ Å$^3$
$Z = 8$
$F(000) = 1328$
$D_x = 1.518$ Mg m$^{-3}$
Melting point: 376 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4972 reflections
$\theta = 2.8–25.0°$
$\mu = 0.43$ mm$^{-1}$
$T = 293$ K
Plate, colourless
0.24 × 0.20 × 0.12 mm

*Data collection*

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ and $\varphi$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.770$, $T_{max} = 1.000$
16038 measured reflections
4972 independent reflections
3759 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.8°$
$h = -15\rightarrow15$
$k = -17\rightarrow17$
$l = -17\rightarrow17$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.098$
$S = 1.04$
4972 reflections
379 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0619P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.30$ e Å$^{-3}$
$\Delta\rho_{min} = -0.31$ e Å$^{-3}$

*Special details*

**Experimental**. IR cm$^{-1}$ (KBr) 3435, 1388; Anal. Calcd for $C_{13}H_{11}ClN_4O_2S$ C, 45.82; H, 2.96; N, 16.44%; Found, C, 45.18; H, 2.92; N, 15.84%.

**Geometry**. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'s involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on $F^2$, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative $F^2$. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on $F^2$ are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1A | 0.20678 (5) | 0.52370 (5) | 0.40718 (5) | 0.06025 (19) |
| Cl1B | 0.93941 (5) | 0.41848 (4) | 0.38570 (5) | 0.05977 (19) |
| S2A | 0.28936 (4) | 0.22270 (3) | 0.58582 (4) | 0.03821 (16) |
| S2B | 0.70463 (4) | 0.13503 (3) | 0.40663 (4) | 0.03622 (15) |
| O3A | 0.26710 (11) | 0.21724 (10) | 0.48964 (11) | 0.0500 (4) |
| O3B | 0.70151 (13) | 0.19837 (10) | 0.47946 (11) | 0.0522 (4) |
| O4A | 0.32556 (11) | 0.14347 (9) | 0.63449 (13) | 0.0562 (5) |
| O4B | 0.63810 (11) | 0.05785 (9) | 0.40271 (11) | 0.0461 (4) |
| N5A | 0.51992 (13) | 0.58429 (10) | 0.64248 (12) | 0.0357 (4) |
| N5B | 0.62508 (13) | 0.45541 (11) | 0.14780 (12) | 0.0369 (4) |
| N6A | 0.30372 (12) | 0.41345 (11) | 0.52175 (12) | 0.0371 (4) |
| N6B | 0.79517 (13) | 0.30202 (11) | 0.33564 (12) | 0.0376 (4) |
| N7A | 0.37871 (13) | 0.29776 (10) | 0.61344 (13) | 0.0439 (5) |
| H7A | 0.4314 | 0.2801 | 0.6480 | 0.053* |
| N7B | 0.67403 (13) | 0.18711 (11) | 0.30975 (12) | 0.0394 (4) |
| H7B | 0.6335 | 0.1599 | 0.2693 | 0.047* |
| N8A | 0.52770 (13) | 0.43954 (10) | 0.69189 (12) | 0.0360 (4) |
| N8B | 0.56595 (12) | 0.31475 (11) | 0.16965 (12) | 0.0364 (4) |
| C9A | 0.17905 (15) | 0.26081 (13) | 0.63400 (15) | 0.0354 (5) |
| C9B | 0.83185 (15) | 0.09728 (13) | 0.40267 (14) | 0.0354 (5) |
| C10A | 0.1679 (2) | 0.23876 (17) | 0.72382 (18) | 0.0609 (7) |
| H10A | 0.2202 | 0.2094 | 0.7593 | 0.073* |
| C10B | 0.91108 (18) | 0.14379 (15) | 0.44983 (16) | 0.0482 (6) |
| H10B | 0.8982 | 0.1949 | 0.4842 | 0.058* |
| C11A | 0.0783 (3) | 0.2610 (2) | 0.7596 (2) | 0.0800 (9) |
| H11A | 0.0695 | 0.2463 | 0.8200 | 0.096* |
| C11B | 1.01033 (19) | 0.11297 (18) | 0.44508 (19) | 0.0594 (7) |
| H11B | 1.0645 | 0.1433 | 0.4771 | 0.071* |
| C12A | 0.0013 (2) | 0.30470 (19) | 0.7073 (2) | 0.0755 (9) |
| H12A | −0.0596 | 0.3187 | 0.7321 | 0.091* |

| | | | | |
|---|---|---|---|---|
| C12B | 1.0294 (2) | 0.03867 (19) | 0.39389 (19) | 0.0615 (7) |
| H12B | 1.0964 | 0.0189 | 0.3909 | 0.074* |
| C13A | 0.01382 (19) | 0.32755 (18) | 0.6197 (2) | 0.0641 (7) |
| H13A | −0.0383 | 0.3579 | 0.5849 | 0.077* |
| C13B | 0.9501 (2) | −0.00710 (18) | 0.34674 (18) | 0.0577 (7) |
| H13B | 0.9635 | −0.0576 | 0.3117 | 0.069* |
| C14A | 0.10334 (16) | 0.30612 (15) | 0.58193 (17) | 0.0458 (6) |
| H14A | 0.1122 | 0.3222 | 0.5219 | 0.055* |
| C14B | 0.85071 (18) | 0.02174 (14) | 0.35123 (16) | 0.0458 (6) |
| H14B | 0.7968 | −0.0094 | 0.3198 | 0.055* |
| C15A | 0.37606 (14) | 0.38857 (12) | 0.58513 (14) | 0.0318 (4) |
| C15B | 0.71004 (15) | 0.27352 (12) | 0.28880 (13) | 0.0321 (5) |
| C16A | 0.30231 (16) | 0.50038 (14) | 0.49461 (15) | 0.0378 (5) |
| C16B | 0.82753 (15) | 0.38663 (14) | 0.32074 (14) | 0.0376 (5) |
| C17A | 0.36691 (15) | 0.56812 (13) | 0.52574 (14) | 0.0356 (5) |
| H17A | 0.3617 | 0.6274 | 0.5041 | 0.043* |
| C17B | 0.78186 (16) | 0.44845 (13) | 0.26077 (14) | 0.0367 (5) |
| H17B | 0.8070 | 0.5069 | 0.2538 | 0.044* |
| C18A | 0.44159 (15) | 0.54000 (12) | 0.59313 (13) | 0.0298 (4) |
| C18B | 0.69432 (14) | 0.41563 (13) | 0.21132 (13) | 0.0317 (4) |
| C19A | 0.44741 (14) | 0.45033 (12) | 0.62405 (13) | 0.0290 (4) |
| C19B | 0.65665 (14) | 0.32852 (12) | 0.22385 (13) | 0.0309 (4) |
| C20A | 0.56688 (17) | 0.52153 (13) | 0.69992 (15) | 0.0386 (5) |
| H20A | 0.6223 | 0.5356 | 0.7415 | 0.046* |
| C20B | 0.55180 (16) | 0.39220 (14) | 0.12623 (15) | 0.0401 (5) |
| H20B | 0.4959 | 0.4029 | 0.0840 | 0.048* |
| C21A | 0.54967 (18) | 0.67998 (13) | 0.63396 (16) | 0.0468 (6) |
| H21A | 0.5035 | 0.7092 | 0.5887 | 0.070* |
| H21B | 0.6182 | 0.6833 | 0.6159 | 0.070* |
| H21C | 0.5467 | 0.7099 | 0.6917 | 0.070* |
| C21B | 0.62941 (19) | 0.54775 (14) | 0.11289 (18) | 0.0530 (6) |
| H21D | 0.6901 | 0.5772 | 0.1399 | 0.080* |
| H21E | 0.5700 | 0.5808 | 0.1280 | 0.080* |
| H21F | 0.6310 | 0.5461 | 0.0477 | 0.080* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1A | 0.0494 (4) | 0.0661 (4) | 0.0616 (4) | 0.0194 (3) | −0.0152 (3) | 0.0047 (3) |
| Cl1B | 0.0511 (4) | 0.0597 (4) | 0.0645 (4) | −0.0155 (3) | −0.0170 (3) | 0.0071 (3) |
| S2A | 0.0297 (3) | 0.0228 (3) | 0.0614 (4) | −0.0001 (2) | −0.0003 (2) | −0.0053 (2) |
| S2B | 0.0421 (3) | 0.0276 (3) | 0.0390 (3) | −0.0011 (2) | 0.0037 (2) | 0.0059 (2) |
| O3A | 0.0468 (9) | 0.0467 (9) | 0.0569 (11) | −0.0055 (7) | 0.0075 (8) | −0.0219 (7) |
| O3B | 0.0701 (11) | 0.0442 (9) | 0.0439 (10) | −0.0004 (8) | 0.0137 (8) | −0.0035 (7) |
| O4A | 0.0366 (8) | 0.0248 (7) | 0.1057 (14) | 0.0018 (6) | −0.0022 (9) | 0.0105 (8) |
| O4B | 0.0462 (9) | 0.0344 (8) | 0.0572 (10) | −0.0067 (7) | 0.0017 (8) | 0.0130 (7) |
| N5A | 0.0416 (10) | 0.0235 (8) | 0.0423 (11) | −0.0050 (7) | 0.0055 (8) | −0.0038 (7) |
| N5B | 0.0379 (10) | 0.0332 (9) | 0.0396 (10) | 0.0005 (8) | 0.0031 (8) | 0.0124 (8) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N6A | 0.0325 (9) | 0.0314 (9) | 0.0467 (11) | 0.0043 (7) | −0.0009 (8) | −0.0028 (8) |
| N6B | 0.0372 (10) | 0.0336 (9) | 0.0413 (11) | −0.0010 (8) | −0.0012 (8) | 0.0063 (7) |
| N7A | 0.0336 (9) | 0.0254 (9) | 0.0695 (14) | −0.0021 (7) | −0.0125 (9) | 0.0058 (8) |
| N7B | 0.0438 (10) | 0.0285 (9) | 0.0437 (11) | −0.0036 (8) | −0.0083 (8) | 0.0071 (7) |
| N8A | 0.0404 (10) | 0.0297 (9) | 0.0372 (10) | −0.0031 (7) | 0.0001 (8) | −0.0019 (7) |
| N8B | 0.0340 (9) | 0.0362 (9) | 0.0387 (10) | −0.0022 (8) | 0.0012 (8) | 0.0083 (8) |
| C9A | 0.0366 (11) | 0.0258 (10) | 0.0434 (13) | −0.0020 (9) | 0.0016 (10) | −0.0051 (9) |
| C9B | 0.0400 (11) | 0.0297 (10) | 0.0356 (12) | −0.0018 (9) | −0.0016 (9) | 0.0104 (9) |
| C10A | 0.0735 (18) | 0.0581 (15) | 0.0509 (17) | 0.0107 (14) | 0.0045 (14) | 0.0047 (12) |
| C10B | 0.0552 (15) | 0.0413 (12) | 0.0451 (14) | −0.0063 (11) | −0.0117 (11) | 0.0010 (10) |
| C11A | 0.112 (3) | 0.075 (2) | 0.059 (2) | 0.0138 (19) | 0.0413 (19) | 0.0038 (15) |
| C11B | 0.0455 (14) | 0.0673 (17) | 0.0621 (18) | −0.0127 (13) | −0.0139 (12) | 0.0145 (14) |
| C12A | 0.070 (2) | 0.0649 (18) | 0.098 (3) | 0.0096 (15) | 0.0439 (19) | −0.0142 (17) |
| C12B | 0.0413 (14) | 0.0714 (18) | 0.072 (2) | 0.0066 (13) | 0.0078 (13) | 0.0200 (15) |
| C13A | 0.0477 (15) | 0.0657 (17) | 0.080 (2) | 0.0208 (13) | 0.0115 (14) | −0.0072 (15) |
| C13B | 0.0556 (16) | 0.0572 (15) | 0.0608 (17) | 0.0078 (13) | 0.0083 (13) | −0.0008 (13) |
| C14A | 0.0399 (12) | 0.0465 (13) | 0.0508 (15) | 0.0105 (10) | 0.0024 (11) | −0.0005 (11) |
| C14B | 0.0480 (14) | 0.0406 (12) | 0.0478 (14) | −0.0033 (10) | −0.0011 (11) | −0.0016 (10) |
| C15A | 0.0319 (10) | 0.0243 (9) | 0.0393 (12) | 0.0022 (8) | 0.0044 (9) | −0.0036 (8) |
| C15B | 0.0335 (11) | 0.0271 (10) | 0.0362 (12) | 0.0017 (9) | 0.0061 (9) | 0.0040 (8) |
| C16A | 0.0350 (11) | 0.0386 (12) | 0.0394 (13) | 0.0117 (10) | 0.0013 (10) | −0.0018 (9) |
| C16B | 0.0346 (11) | 0.0399 (12) | 0.0381 (13) | −0.0043 (9) | 0.0028 (9) | 0.0002 (9) |
| C17A | 0.0401 (11) | 0.0287 (10) | 0.0394 (12) | 0.0078 (9) | 0.0106 (10) | 0.0025 (9) |
| C17B | 0.0390 (11) | 0.0317 (10) | 0.0400 (13) | −0.0066 (9) | 0.0065 (10) | 0.0053 (9) |
| C18A | 0.0345 (11) | 0.0264 (10) | 0.0301 (11) | 0.0021 (8) | 0.0117 (9) | −0.0037 (8) |
| C18B | 0.0344 (10) | 0.0299 (10) | 0.0318 (11) | 0.0005 (9) | 0.0092 (9) | 0.0065 (8) |
| C19A | 0.0310 (10) | 0.0269 (10) | 0.0297 (11) | 0.0007 (8) | 0.0063 (9) | −0.0019 (8) |
| C19B | 0.0306 (10) | 0.0298 (10) | 0.0330 (12) | 0.0012 (8) | 0.0066 (9) | 0.0024 (8) |
| C20A | 0.0412 (12) | 0.0351 (11) | 0.0379 (13) | −0.0038 (9) | −0.0044 (10) | −0.0052 (9) |
| C20B | 0.0350 (11) | 0.0429 (12) | 0.0412 (13) | −0.0033 (10) | −0.0034 (10) | 0.0116 (10) |
| C21A | 0.0570 (14) | 0.0276 (11) | 0.0568 (15) | −0.0101 (10) | 0.0108 (12) | −0.0030 (10) |
| C21B | 0.0605 (15) | 0.0373 (12) | 0.0606 (16) | −0.0016 (11) | 0.0013 (13) | 0.0230 (11) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cl1A—C16A | 1.746 (2) | C10B—C11B | 1.385 (3) |
| Cl1B—C16B | 1.741 (2) | C10B—H10B | 0.9300 |
| S2A—O3A | 1.4198 (17) | C11A—C12A | 1.373 (4) |
| S2A—O4A | 1.4273 (15) | C11A—H11A | 0.9300 |
| S2A—N7A | 1.6347 (17) | C11B—C12B | 1.363 (4) |
| S2A—C9A | 1.757 (2) | C11B—H11B | 0.9300 |
| S2B—O3B | 1.4230 (16) | C12A—C13A | 1.354 (4) |
| S2B—O4B | 1.4305 (14) | C12A—H12A | 0.9300 |
| S2B—N7B | 1.6352 (17) | C12B—C13B | 1.373 (4) |
| S2B—C9B | 1.763 (2) | C12B—H12B | 0.9300 |
| N5A—C20A | 1.361 (3) | C13A—C14A | 1.379 (3) |
| N5A—C18A | 1.368 (2) | C13A—H13A | 0.9300 |
| N5A—C21A | 1.470 (2) | C13B—C14B | 1.377 (3) |

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|---|---|---|---|
| N5B—C20B | 1.354 (3) | C13B—H13B | 0.9300 |
| N5B—C18B | 1.374 (2) | C14A—H14A | 0.9300 |
| N5B—C21B | 1.456 (2) | C14B—H14B | 0.9300 |
| N6A—C15A | 1.320 (2) | C15A—C19A | 1.390 (3) |
| N6A—C16A | 1.341 (3) | C15B—C19B | 1.392 (3) |
| N6B—C15B | 1.326 (3) | C16A—C17A | 1.361 (3) |
| N6B—C16B | 1.340 (2) | C16B—C17B | 1.367 (3) |
| N7A—C15A | 1.400 (2) | C17A—C18A | 1.392 (3) |
| N7A—H7A | 0.8600 | C17A—H17A | 0.9300 |
| N7B—C15B | 1.401 (2) | C17B—C18B | 1.389 (3) |
| N7B—H7B | 0.8600 | C17B—H17B | 0.9300 |
| N8A—C20A | 1.313 (2) | C18A—C19A | 1.396 (3) |
| N8A—C19A | 1.392 (3) | C18B—C19B | 1.393 (3) |
| N8B—C20B | 1.312 (2) | C20A—H20A | 0.9300 |
| N8B—C19B | 1.385 (2) | C20B—H20B | 0.9300 |
| C9A—C14A | 1.371 (3) | C21A—H21A | 0.9600 |
| C9A—C10A | 1.380 (3) | C21A—H21B | 0.9600 |
| C9B—C10B | 1.378 (3) | C21A—H21C | 0.9600 |
| C9B—C14B | 1.380 (3) | C21B—H21D | 0.9600 |
| C10A—C11A | 1.369 (4) | C21B—H21E | 0.9600 |
| C10A—H10A | 0.9300 | C21B—H21F | 0.9600 |

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|---|---|---|---|
| O3A—S2A—O4A | 118.82 (10) | C12B—C13B—H13B | 120.0 |
| O3A—S2A—N7A | 111.37 (10) | C14B—C13B—H13B | 120.0 |
| O4A—S2A—N7A | 103.28 (9) | C9A—C14A—C13A | 119.1 (2) |
| O3A—S2A—C9A | 108.41 (10) | C9A—C14A—H14A | 120.5 |
| O4A—S2A—C9A | 107.92 (10) | C13A—C14A—H14A | 120.5 |
| N7A—S2A—C9A | 106.31 (9) | C9B—C14B—C13B | 119.4 (2) |
| O3B—S2B—O4B | 119.51 (9) | C9B—C14B—H14B | 120.3 |
| O3B—S2B—N7B | 109.03 (9) | C13B—C14B—H14B | 120.3 |
| O4B—S2B—N7B | 103.68 (9) | N6A—C15A—C19A | 121.52 (17) |
| O3B—S2B—C9B | 108.80 (10) | N6A—C15A—N7A | 118.16 (17) |
| O4B—S2B—C9B | 108.84 (9) | C19A—C15A—N7A | 120.32 (18) |
| N7B—S2B—C9B | 106.16 (9) | N6B—C15B—C19B | 121.33 (17) |
| C20A—N5A—C18A | 106.34 (15) | N6B—C15B—N7B | 117.25 (17) |
| C20A—N5A—C21A | 126.50 (18) | C19B—C15B—N7B | 121.38 (18) |
| C18A—N5A—C21A | 127.14 (18) | N6A—C16A—C17A | 127.47 (19) |
| C20B—N5B—C18B | 106.11 (15) | N6A—C16A—Cl1A | 113.37 (16) |
| C20B—N5B—C21B | 127.47 (19) | C17A—C16A—Cl1A | 119.14 (16) |
| C18B—N5B—C21B | 126.40 (18) | N6B—C16B—C17B | 126.69 (19) |
| C15A—N6A—C16A | 117.71 (17) | N6B—C16B—Cl1B | 115.09 (16) |
| C15B—N6B—C16B | 118.25 (18) | C17B—C16B—Cl1B | 118.22 (15) |
| C15A—N7A—S2A | 125.03 (15) | C16A—C17A—C18A | 113.45 (18) |
| C15A—N7A—H7A | 117.5 | C16A—C17A—H17A | 123.3 |
| S2A—N7A—H7A | 117.5 | C18A—C17A—H17A | 123.3 |
| C15B—N7B—S2B | 123.79 (15) | C16B—C17B—C18B | 113.53 (18) |
| C15B—N7B—H7B | 118.1 | C16B—C17B—H17B | 123.2 |
| S2B—N7B—H7B | 118.1 | C18B—C17B—H17B | 123.2 |

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|---|---|---|---|
| C20A—N8A—C19A | 102.94 (16) | N5A—C18A—C17A | 133.00 (17) |
| C20B—N8B—C19B | 103.25 (16) | N5A—C18A—C19A | 105.18 (17) |
| C14A—C9A—C10A | 121.0 (2) | C17A—C18A—C19A | 121.82 (18) |
| C14A—C9A—S2A | 120.72 (17) | N5B—C18B—C17B | 132.22 (17) |
| C10A—C9A—S2A | 118.14 (18) | N5B—C18B—C19B | 105.20 (17) |
| C10B—C9B—C14B | 120.8 (2) | C17B—C18B—C19B | 122.51 (18) |
| C10B—C9B—S2B | 119.93 (17) | N8A—C19A—C15A | 131.09 (17) |
| C14B—C9B—S2B | 119.24 (16) | N8A—C19A—C18A | 110.89 (17) |
| C11A—C10A—C9A | 118.7 (3) | C15A—C19A—C18A | 118.02 (18) |
| C11A—C10A—H10A | 120.7 | N8B—C19B—C18B | 110.79 (17) |
| C9A—C10A—H10A | 120.7 | N8B—C19B—C15B | 131.45 (17) |
| C9B—C10B—C11B | 118.7 (2) | C18B—C19B—C15B | 117.66 (18) |
| C9B—C10B—H10B | 120.6 | N8A—C20A—N5A | 114.65 (19) |
| C11B—C10B—H10B | 120.6 | N8A—C20A—H20A | 122.7 |
| C10A—C11A—C12A | 120.6 (3) | N5A—C20A—H20A | 122.7 |
| C10A—C11A—H11A | 119.7 | N8B—C20B—N5B | 114.65 (18) |
| C12A—C11A—H11A | 119.7 | N8B—C20B—H20B | 122.7 |
| C12B—C11B—C10B | 120.6 (2) | N5B—C20B—H20B | 122.7 |
| C12B—C11B—H11B | 119.7 | N5A—C21A—H21A | 109.5 |
| C10B—C11B—H11B | 119.7 | N5A—C21A—H21B | 109.5 |
| C13A—C12A—C11A | 120.2 (2) | H21A—C21A—H21B | 109.5 |
| C13A—C12A—H12A | 119.9 | N5A—C21A—H21C | 109.5 |
| C11A—C12A—H12A | 119.9 | H21A—C21A—H21C | 109.5 |
| C11B—C12B—C13B | 120.3 (2) | H21B—C21A—H21C | 109.5 |
| C11B—C12B—H12B | 119.8 | N5B—C21B—H21D | 109.5 |
| C13B—C12B—H12B | 119.8 | N5B—C21B—H21E | 109.5 |
| C12A—C13A—C14A | 120.4 (3) | H21D—C21B—H21E | 109.5 |
| C12A—C13A—H13A | 119.8 | N5B—C21B—H21F | 109.5 |
| C14A—C13A—H13A | 119.8 | H21D—C21B—H21F | 109.5 |
| C12B—C13B—C14B | 120.0 (2) | H21E—C21B—H21F | 109.5 |

| | | | |
|---|---|---|---|
| O3A—S2A—N7A—C15A | 54.0 (2) | C15B—N6B—C16B—C17B | −0.4 (3) |
| O4A—S2A—N7A—C15A | −177.38 (17) | C15B—N6B—C16B—Cl1B | 179.63 (15) |
| C9A—S2A—N7A—C15A | −63.9 (2) | N6A—C16A—C17A—C18A | 0.2 (3) |
| O3B—S2B—N7B—C15B | 42.58 (18) | Cl1A—C16A—C17A—C18A | −177.92 (14) |
| O4B—S2B—N7B—C15B | 170.92 (16) | N6B—C16B—C17B—C18B | −1.1 (3) |
| C9B—S2B—N7B—C15B | −74.47 (18) | Cl1B—C16B—C17B—C18B | 178.91 (15) |
| O3A—S2A—C9A—C14A | −20.6 (2) | C20A—N5A—C18A—C17A | 179.0 (2) |
| O4A—S2A—C9A—C14A | −150.49 (17) | C21A—N5A—C18A—C17A | −2.4 (3) |
| N7A—S2A—C9A—C14A | 99.25 (18) | C20A—N5A—C18A—C19A | −0.8 (2) |
| O3A—S2A—C9A—C10A | 155.31 (17) | C21A—N5A—C18A—C19A | 177.74 (17) |
| O4A—S2A—C9A—C10A | 25.4 (2) | C16A—C17A—C18A—N5A | −179.73 (19) |
| N7A—S2A—C9A—C10A | −84.85 (19) | C16A—C17A—C18A—C19A | 0.1 (3) |
| O3B—S2B—C9B—C10B | −14.6 (2) | C20B—N5B—C18B—C17B | −176.7 (2) |
| O4B—S2B—C9B—C10B | −146.40 (17) | C21B—N5B—C18B—C17B | 2.1 (3) |
| N7B—S2B—C9B—C10B | 102.56 (18) | C20B—N5B—C18B—C19B | 0.0 (2) |
| O3B—S2B—C9B—C14B | 166.09 (16) | C21B—N5B—C18B—C19B | 178.77 (19) |
| O4B—S2B—C9B—C14B | 34.3 (2) | C16B—C17B—C18B—N5B | 177.4 (2) |

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|---|---|---|---|
| N7B—S2B—C9B—C14B | −76.70 (18) | C16B—C17B—C18B—C19B | 1.2 (3) |
| C14A—C9A—C10A—C11A | 1.7 (4) | C20A—N8A—C19A—C15A | −179.5 (2) |
| S2A—C9A—C10A—C11A | −174.2 (2) | C20A—N8A—C19A—C18A | 0.2 (2) |
| C14B—C9B—C10B—C11B | −0.4 (3) | N6A—C15A—C19A—N8A | 178.71 (19) |
| S2B—C9B—C10B—C11B | −179.61 (18) | N7A—C15A—C19A—N8A | −0.5 (3) |
| C9A—C10A—C11A—C12A | −0.3 (4) | N6A—C15A—C19A—C18A | −1.0 (3) |
| C9B—C10B—C11B—C12B | 0.7 (4) | N7A—C15A—C19A—C18A | 179.78 (17) |
| C10A—C11A—C12A—C13A | −0.9 (5) | N5A—C18A—C19A—N8A | 0.4 (2) |
| C10B—C11B—C12B—C13B | −0.5 (4) | C17A—C18A—C19A—N8A | −179.47 (17) |
| C11A—C12A—C13A—C14A | 0.8 (4) | N5A—C18A—C19A—C15A | −179.87 (16) |
| C11B—C12B—C13B—C14B | −0.2 (4) | C17A—C18A—C19A—C15A | 0.3 (3) |
| C10A—C9A—C14A—C13A | −1.7 (3) | C20B—N8B—C19B—C18B | 0.4 (2) |
| S2A—C9A—C14A—C13A | 174.03 (18) | C20B—N8B—C19B—C15B | 176.6 (2) |
| C12A—C13A—C14A—C9A | 0.5 (4) | N5B—C18B—C19B—N8B | −0.3 (2) |
| C10B—C9B—C14B—C13B | −0.3 (3) | C17B—C18B—C19B—N8B | 176.86 (18) |
| S2B—C9B—C14B—C13B | 178.94 (18) | N5B—C18B—C19B—C15B | −177.09 (17) |
| C12B—C13B—C14B—C9B | 0.6 (4) | C17B—C18B—C19B—C15B | 0.0 (3) |
| C16A—N6A—C15A—C19A | 1.2 (3) | N6B—C15B—C19B—N8B | −177.66 (19) |
| C16A—N6A—C15A—N7A | −179.50 (18) | N7B—C15B—C19B—N8B | 0.0 (3) |
| S2A—N7A—C15A—N6A | −9.7 (3) | N6B—C15B—C19B—C18B | −1.6 (3) |
| S2A—N7A—C15A—C19A | 169.53 (15) | N7B—C15B—C19B—C18B | 176.01 (17) |
| C16B—N6B—C15B—C19B | 1.8 (3) | C19A—N8A—C20A—N5A | −0.8 (2) |
| C16B—N6B—C15B—N7B | −175.93 (17) | C18A—N5A—C20A—N8A | 1.1 (2) |
| S2B—N7B—C15B—N6B | 21.4 (2) | C21A—N5A—C20A—N8A | −177.51 (18) |
| S2B—N7B—C15B—C19B | −156.28 (15) | C19B—N8B—C20B—N5B | −0.4 (2) |
| C15A—N6A—C16A—C17A | −0.9 (3) | C18B—N5B—C20B—N8B | 0.2 (2) |
| C15A—N6A—C16A—Cl1A | 177.34 (15) | C21B—N5B—C20B—N8B | −178.51 (19) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N7*A*—H7*A*···N8*B*$^{i}$ | 0.86 | 2.25 | 3.014 (2) | 148 |
| N7*B*—H7*B*···N8*A*$^{ii}$ | 0.86 | 2.25 | 3.092 (2) | 165 |
| C13*A*—H13*A*···Cl1*A*$^{iii}$ | 0.93 | 2.82 | 3.620 (3) | 144 |
| C20*A*—H20*A*···O4*A*$^{iv}$ | 0.93 | 2.47 | 3.243 (3) | 141 |

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