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# 4-{2-[5-(4-Chlorophenyl)-1-(4-fluorophenyl)-1*H*-pyrazol-3-yl]thiazol-4-yl}benzonitrile

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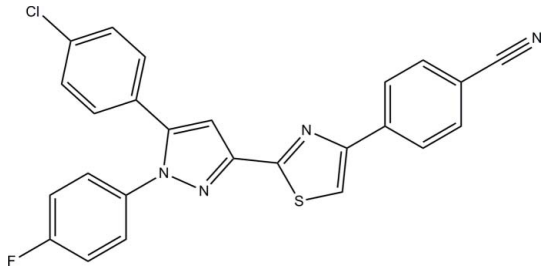
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.042; $wR$ factor = 0.107; data-to-parameter ratio = 21.8.

The asymmetric unit of the title compound, $C_{25}H_{14}ClFN_4S$, contains two independent molecules (*A* and *B*). Each molecule consists of five rings, namely chlorophenyl, fluorophenyl, 1*H*-pyrazole, thiazole and benzonitrile. In molecule *A*, the 1*H*-pyrazole ring makes dihedral angles of 52.54 (8), 35.96 (8) and 15.43 (8)° with respect to the attached chlorophenyl, fluorophenyl and thiazole rings. The corresponding values in molecule *B* are 51.65 (8), 37.26 (8) and 8.32 (8)°. In the crystal, molecules are linked into dimers by C—H···N hydrogen bonds, generating $R_2^2(10)$ ring motifs. These dimers are further linked into two-dimensional arrays parallel to the *ab* plane *via* intermolecular weak C—H···N and C—H···F hydrogen bonds. The crystal structure is further stabilized by weak $\pi$-$\pi$ interactions [with centroid–centroid distances of 3.4303 (9) and 3.6826 (9) Å] and weak C—H···$\pi$ interactions.

## Related literature

For background and the microbial activity of pyrazole derivatives, see: Ragavan *et al.* (2009, 2010). For related structures, see: Shahani *et al.* (2009, 2010*a*,*b*). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For standard bond-length data, see: Allen *et al.* (1987). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986).




## Experimental

### Crystal data

$C_{25}H_{14}ClFN_4S$
$M_r$ = 456.91
Triclinic, $P\overline{1}$
$a$ = 10.1412 (9) Å
$b$ = 15.0496 (14) Å
$c$ = 15.8890 (14) Å
$\alpha$ = 105.518 (2)°
$\beta$ = 107.869 (2)°
$\gamma$ = 99.253 (2)°
$V$ = 2144.5 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.31 mm$^{-1}$
$T$ = 100 K
0.32 × 0.26 × 0.08 mm

### Data collection

Bruker APEXII DUO CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.909, $T_{max}$ = 0.977
44680 measured reflections
12570 independent reflections
9300 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.047

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.107
$S$ = 1.01
12570 reflections
577 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.45 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.50 e Å$^{-3}$

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

*Cg*1 and *Cg*2 are the centroids of the C1*A*–C6*A* and C1*B*–C6*B* rings, respectively.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C5*A*—H5*AA*···F1*A*$^{i}$ | 0.93 | 2.39 | 3.149 (2) | 138 |
| C8*B*—H8*BA*···F1*B*$^{i}$ | 0.93 | 2.42 | 3.283 (2) | 154 |
| C17*B*—H17*A*···N4*A*$^{ii}$ | 0.93 | 2.54 | 3.419 (2) | 159 |
| C17*A*—H17*B*···N4*B*$^{ii}$ | 0.93 | 2.58 | 3.453 (2) | 156 |
| C25*B*—H25*A*···N2*A*$^{iii}$ | 0.93 | 2.53 | 3.457 (2) | 175 |
| C24*A*—H24*B*···*Cg*1$^{iv}$ | 0.93 | 2.96 | 3.7811 (18) | 148 |
| C21*B*—H21*A*···*Cg*2$^{v}$ | 0.93 | 2.97 | 3.6423 (19) | 131 |

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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‡ Thomson Reuters ResearcherID: A-3561-2009.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5111).

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# supporting information

*Acta Cryst.* (2010). E**66**, o2286–o2287 [https://doi.org/10.1107/S1600536810031405]

## 4-{2-[5-(4-Chlorophenyl)-1-(4-fluorophenyl)-1*H*-pyrazol-3-yl]thiazol-4-yl}benzonitrile

**Tara Shahani, Hoong-Kun Fun, R. Venkat Ragavan, V. Vijayakumar and S. Sarveswari**

### S1. Comment

Antibacterial and antifungal activities of the azoles are most widely studied and some of them are used clinically as antimicrobial agents. In particular pyrazole derivatives are extensively studied and used as antimicrobial agents. However, azole-resistant strains led to the development of new antimicrobial compounds. Pyrazole is an important class of heterocyclic compounds and many pyrazole derivatives are reported to have a broad spectrum of biological activities, such as anti-inflammatory, antifungal, herbicidal, anti-tumour, cytotoxic and antiviral activities. Pyrazole derivatives also act as antiangiogenic agents, A3 adenosine receptor antagonists, neuropeptide YY5 receptor antagonists as well as kinase inhibitor for treatment of type 2 diabetes, hyperlipidemia, obesity, and thrombopiotinmimetics. Recently urea derivatives of pyrazoles have been reported as potent inhibitors of p38 kinase. Since the high electronegativity of halogens (particularly chlorine and fluorine) in the aromatic part of the drug molecules play an important role in enhancing their biological activity, we are interested to have 4-fluoro or 4-chloro substitution in the aryls of 1,5-diaryl pyrazoles. As part of our ongoing research aiming on the synthesis of new antimicrobial compounds, we have reported the synthesis of novel pyrazole derivatives and their microbial activities (Ragavan *et al.*, 2009; 2010).

The asymmetric unit of the title compound (Fig. 1) contains two molecules (*A* and *B*) with similar geometries. Each molecule consists of five rings, namely chlorophenyl (C1–C6/Cl1), fluorophenyl (C20–C25/F1), 1*H*-pyrazole (N1/N2/C7–C9), thiazole (N3/S1/C10–C12) and benzonitrile (C13–C19/N4) rings. In molecule *A*, the 1*H*-pyrazole ring is inclined at angles of 52.54 (8) and 35.96 (8)° and 15.43 (8)° with respect to the chlorophenyl, fluorophenyl and thiazole rings attached to it. The corresponding values in molecule *B* are 51.65 (8), 37.26 (8) and 8.32 (8)°. The bond lengths (Allen *et al.*, 1987), and angles are within normal ranges and comparable to the closely related structures (Shahani *et al.*,2009; 2010*a*,*b*).

In the crystal packing (Fig. 2), intermolecular C17B—H17A···N4A and C17A—H17B···N4B hydrogen bonds (Table 1) link the neighbouring molecules into dimers, generating $R^2_2(10)$ ring motifs (Bernstein *et al.*, 1995). These dimers are further linked into two-dimensional arrays parallel to the *ab* plane by intermolecular C5A—H5AA···F1A, C8B—H8BA···F1B and C25B—H25A···N2A hydrogen bonds (Table 1). Weak $\pi\cdots\pi$ interactions are observed [$Cg1\cdots Cg1^{vi}$ = 3.4303 (9) Å, symmetry code vi = 2 - *x*, 2 - *y*, 1 - *z*], [$Cg1\cdots Cg2^{vii}$ = 3.6826 (9) Å, symmetry code vii = *x*, 1 + *y*, *z*] where *Cg*1 is the centroid of the thiazole ring (S1A/N3A/C10A—C12A) and *Cg*2 is the centroid of the 1*H*-pyrazole ring (N1B/N2B/C7B–C9B). The crystal structure is further stabilized by C—H···$\pi$ interactions (Table 1), involving the C1A–C6A (centroid *Cg*3) and C1B–C6B rings (centroid *Cg*4).

## S2. Experimental

The compound has been synthesized by adopting the procedure available in the literature and purified by crystallization in ethanol (Ragavan *et al.*, 2009; 2010). Yellow solid, 76% yield, *mp*: 479.9–480.8 k.

## S3. Refinement

H atoms were positioned geometrically [C–H = 0.9300 Å] and refined using a riding model, with $U_{iso}$(H) = 1.2 $U_{eq}$(C).

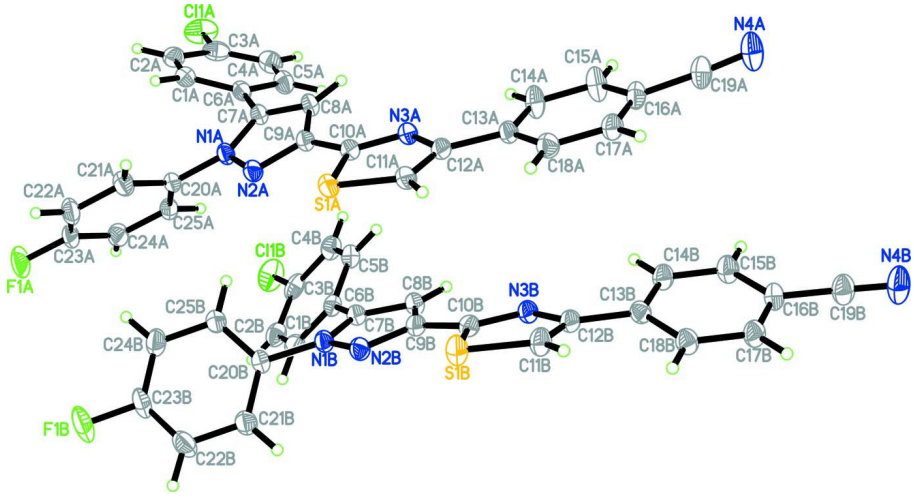


**Figure 1**

The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atom numbering scheme.

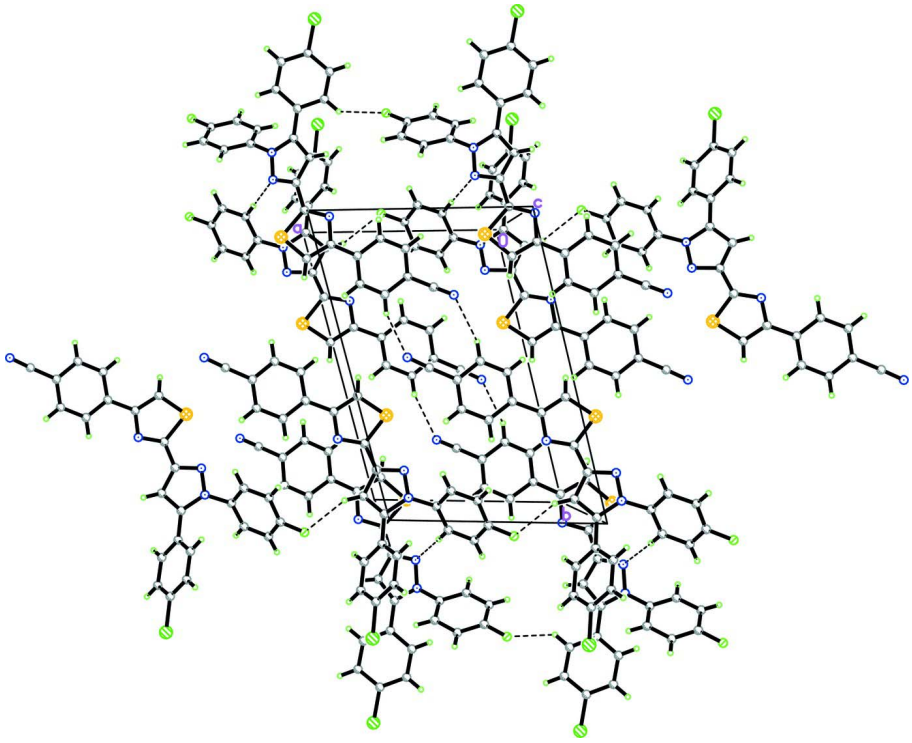

**Figure 2**

The crystal packing of the title compound, showing a two-dimensional array parallel to the *ab* plane. Intermolecular hydrogen bonds are shown as dashed lines.

**4-{2-[5-(4-Chlorophenyl)-1-(4-fluorophenyl)-1*H*-pyrazol-3-yl]thiazol- 4-yl}benzonitrile**

*Crystal data*

$C_{25}H_{14}ClFN_4S$
$M_r = 456.91$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 10.1412\ (9)$ Å
$b = 15.0496\ (14)$ Å
$c = 15.8890\ (14)$ Å
$\alpha = 105.518\ (2)°$
$\beta = 107.869\ (2)°$
$\gamma = 99.253\ (2)°$
$V = 2144.5\ (3)$ Å$^3$
$Z = 4$
$F(000) = 936$
$D_x = 1.415$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8583 reflections
$\theta = 2.7–30.0°$
$\mu = 0.31$ mm$^{-1}$
$T = 100$ K
Plate, yellow
0.32 × 0.26 × 0.08 mm

*Data collection*

Bruker APEXII DUO CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min} = 0.909$, $T_{max} = 0.977$
44680 measured reflections
12570 independent reflections
9300 reflections with $I > 2\sigma(I)$
$R_{int} = 0.047$
$\theta_{max} = 30.2°$, $\theta_{min} = 1.7°$
$h = -14\rightarrow14$
$k = -21\rightarrow21$
$l = -22\rightarrow22$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.107$
$S = 1.01$
12570 reflections
577 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
$w = 1/[\sigma^2(F_o^2) + (0.044P)^2 + 0.5673P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.45$ e Å$^{-3}$
$\Delta\rho_{min} = -0.50$ e Å$^{-3}$

*Special details*

**Experimental**. The crystal was placed in the cold stream of an Oxford Cyrosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'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 $F^2 > \sigma(F^2)$ 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 | 0.65750 (6) | 0.27225 (3) | 0.07240 (3) | 0.04616 (13) |
| S1A | 1.13306 (4) | 1.04182 (3) | 0.40859 (3) | 0.02482 (8) |
| F1A | 1.42149 (12) | 0.59713 (9) | 0.08545 (7) | 0.0464 (3) |
| N1A | 1.06028 (13) | 0.73997 (8) | 0.25101 (9) | 0.0217 (2) |
| N2A | 1.09248 (13) | 0.83652 (8) | 0.29256 (9) | 0.0229 (3) |
| N3A | 0.86452 (14) | 0.97158 (9) | 0.37237 (9) | 0.0233 (3) |
| N4A | 0.37277 (16) | 1.24996 (10) | 0.53307 (12) | 0.0402 (4) |
| C1A | 0.95272 (17) | 0.52359 (11) | 0.21546 (11) | 0.0248 (3) |
| H1AA | 1.0519 | 0.5452 | 0.2463 | 0.030* |
| C2A | 0.88712 (18) | 0.42599 (11) | 0.17403 (11) | 0.0284 (3) |
| H2AA | 0.9423 | 0.3823 | 0.1763 | 0.034* |
| C3A | 0.73902 (19) | 0.39404 (11) | 0.12930 (11) | 0.0312 (4) |
| C4A | 0.65433 (18) | 0.45760 (12) | 0.12679 (12) | 0.0324 (4) |
| H4AA | 0.5548 | 0.4354 | 0.0986 | 0.039* |
| C5A | 0.72013 (17) | 0.55472 (12) | 0.16696 (11) | 0.0290 (3) |
| H5AA | 0.6640 | 0.5979 | 0.1648 | 0.035* |
| C6A | 0.87003 (16) | 0.58924 (10) | 0.21090 (10) | 0.0229 (3) |
| C7A | 0.93212 (15) | 0.69361 (10) | 0.25151 (10) | 0.0220 (3) |
| C8A | 0.88014 (16) | 0.76421 (11) | 0.29533 (11) | 0.0242 (3) |
| H8AA | 0.7953 | 0.7563 | 0.3069 | 0.029* |
| C9A | 0.98191 (16) | 0.85051 (10) | 0.31872 (10) | 0.0222 (3) |
| C10A | 0.97933 (16) | 0.94805 (10) | 0.36358 (10) | 0.0225 (3) |
| C11A | 1.03671 (16) | 1.11797 (11) | 0.44212 (10) | 0.0241 (3) |

| | | | | |
|---|---|---|---|---|
| H11A | 1.0741 | 1.1836 | 0.4728 | 0.029* |
| C12A | 0.89653 (16) | 1.06938 (10) | 0.41774 (10) | 0.0227 (3) |
| C13A | 0.78227 (16) | 1.11019 (10) | 0.43729 (10) | 0.0231 (3) |
| C14A | 0.64515 (18) | 1.05103 (12) | 0.41109 (12) | 0.0331 (4) |
| H14B | 0.6257 | 0.9860 | 0.3792 | 0.040* |
| C15A | 0.53762 (18) | 1.08749 (12) | 0.43178 (13) | 0.0357 (4) |
| H15B | 0.4465 | 1.0473 | 0.4135 | 0.043* |
| C16A | 0.56653 (17) | 1.18491 (11) | 0.48025 (11) | 0.0275 (3) |
| C17A | 0.70275 (18) | 1.24542 (11) | 0.50599 (11) | 0.0283 (3) |
| H17B | 0.7219 | 1.3105 | 0.5376 | 0.034* |
| C18A | 0.80874 (18) | 1.20810 (11) | 0.48427 (11) | 0.0276 (3) |
| H18B | 0.8990 | 1.2486 | 0.5011 | 0.033* |
| C19A | 0.45761 (17) | 1.22203 (11) | 0.50766 (12) | 0.0311 (4) |
| C20A | 1.15274 (15) | 0.70276 (10) | 0.20723 (10) | 0.0211 (3) |
| C21A | 1.29851 (17) | 0.72700 (12) | 0.25942 (11) | 0.0282 (3) |
| H21B | 1.3348 | 0.7669 | 0.3218 | 0.034* |
| C22A | 1.39029 (18) | 0.69147 (13) | 0.21811 (12) | 0.0333 (4) |
| H22B | 1.4884 | 0.7068 | 0.2521 | 0.040* |
| C23A | 1.33238 (18) | 0.63320 (13) | 0.12600 (12) | 0.0310 (4) |
| C24A | 1.18802 (18) | 0.60842 (12) | 0.07246 (11) | 0.0294 (3) |
| H24B | 1.1524 | 0.5684 | 0.0102 | 0.035* |
| C25A | 1.09718 (16) | 0.64470 (11) | 0.11382 (10) | 0.0243 (3) |
| H25B | 0.9995 | 0.6302 | 0.0790 | 0.029* |
| Cl1B | 0.76527 (5) | −0.39437 (3) | −0.11384 (3) | 0.04333 (12) |
| S1B | 1.14106 (4) | 0.33994 (3) | 0.36702 (3) | 0.02914 (9) |
| F1B | 1.57725 (11) | −0.05590 (8) | 0.10753 (9) | 0.0484 (3) |
| N1B | 1.13119 (13) | 0.06398 (8) | 0.18871 (9) | 0.0212 (2) |
| N2B | 1.14761 (13) | 0.15432 (8) | 0.24368 (9) | 0.0224 (2) |
| N3B | 0.86803 (13) | 0.25950 (8) | 0.29038 (8) | 0.0216 (2) |
| N4B | 0.31537 (16) | 0.53818 (10) | 0.35928 (12) | 0.0417 (4) |
| C1B | 0.99178 (17) | −0.12120 (11) | 0.01556 (10) | 0.0251 (3) |
| H1BA | 1.0637 | −0.0792 | 0.0097 | 0.030* |
| C2B | 0.93788 (18) | −0.21482 (11) | −0.04635 (11) | 0.0286 (3) |
| H2BA | 0.9740 | −0.2358 | −0.0931 | 0.034* |
| C3B | 0.82978 (18) | −0.27638 (11) | −0.03761 (11) | 0.0287 (3) |
| C4B | 0.77397 (17) | −0.24687 (11) | 0.03145 (12) | 0.0284 (3) |
| H4BA | 0.7011 | −0.2890 | 0.0363 | 0.034* |
| C5B | 0.82882 (16) | −0.15338 (10) | 0.09319 (11) | 0.0246 (3) |
| H5BA | 0.7920 | −0.1328 | 0.1397 | 0.029* |
| C6B | 0.93883 (16) | −0.08956 (10) | 0.08655 (10) | 0.0220 (3) |
| C7B | 0.99122 (16) | 0.00952 (10) | 0.15263 (10) | 0.0212 (3) |
| C8B | 0.91412 (16) | 0.06778 (10) | 0.18710 (10) | 0.0230 (3) |
| H8BA | 0.8164 | 0.0520 | 0.1760 | 0.028* |
| C9B | 1.01516 (16) | 0.15581 (10) | 0.24242 (10) | 0.0219 (3) |
| C10B | 0.99350 (16) | 0.24426 (10) | 0.29498 (10) | 0.0218 (3) |
| C11B | 1.02670 (17) | 0.40573 (11) | 0.39097 (11) | 0.0267 (3) |
| H11B | 1.0558 | 0.4691 | 0.4303 | 0.032* |
| C12B | 0.88655 (16) | 0.35308 (10) | 0.34484 (10) | 0.0220 (3) |

| | | | | |
|---|---|---|---|---|
| C13B | 0.76062 (16) | 0.38949 (10) | 0.34638 (10) | 0.0217 (3) |
| C14B | 0.62431 (17) | 0.32800 (10) | 0.31896 (11) | 0.0255 (3) |
| H14A | 0.6121 | 0.2622 | 0.2988 | 0.031* |
| C15B | 0.50724 (17) | 0.36374 (11) | 0.32137 (12) | 0.0289 (3) |
| H15A | 0.4171 | 0.3223 | 0.3030 | 0.035* |
| C16B | 0.52600 (17) | 0.46296 (11) | 0.35171 (11) | 0.0258 (3) |
| C17B | 0.66100 (17) | 0.52504 (10) | 0.37804 (11) | 0.0262 (3) |
| H17A | 0.6732 | 0.5908 | 0.3977 | 0.031* |
| C18B | 0.77587 (17) | 0.48827 (10) | 0.37473 (11) | 0.0252 (3) |
| H18A | 0.8654 | 0.5298 | 0.3916 | 0.030* |
| C19B | 0.40724 (18) | 0.50352 (11) | 0.35543 (12) | 0.0314 (4) |
| C20B | 1.25363 (15) | 0.03680 (10) | 0.17432 (10) | 0.0216 (3) |
| C21B | 1.33796 (17) | 0.09201 (11) | 0.14291 (12) | 0.0284 (3) |
| H21A | 1.3194 | 0.1487 | 0.1358 | 0.034* |
| C22B | 1.45039 (18) | 0.06178 (12) | 0.12222 (14) | 0.0355 (4) |
| H22A | 1.5097 | 0.0982 | 0.1023 | 0.043* |
| C23B | 1.47150 (17) | −0.02352 (12) | 0.13207 (13) | 0.0321 (4) |
| C24B | 1.39172 (17) | −0.07789 (11) | 0.16568 (12) | 0.0303 (3) |
| H24A | 1.4112 | −0.1342 | 0.1731 | 0.036* |
| C25B | 1.28151 (16) | −0.04656 (11) | 0.18819 (11) | 0.0258 (3) |
| H25A | 1.2270 | −0.0810 | 0.2123 | 0.031* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1A | 0.0592 (3) | 0.0278 (2) | 0.0379 (2) | −0.0061 (2) | 0.0127 (2) | 0.00634 (18) |
| S1A | 0.02376 (18) | 0.02641 (18) | 0.02893 (19) | 0.00997 (14) | 0.01377 (15) | 0.00987 (15) |
| F1A | 0.0419 (6) | 0.0755 (8) | 0.0383 (6) | 0.0401 (6) | 0.0251 (5) | 0.0185 (6) |
| N1A | 0.0211 (6) | 0.0218 (6) | 0.0257 (6) | 0.0092 (5) | 0.0124 (5) | 0.0070 (5) |
| N2A | 0.0248 (6) | 0.0218 (6) | 0.0264 (6) | 0.0097 (5) | 0.0134 (5) | 0.0082 (5) |
| N3A | 0.0255 (6) | 0.0244 (6) | 0.0252 (6) | 0.0113 (5) | 0.0133 (5) | 0.0092 (5) |
| N4A | 0.0261 (7) | 0.0277 (7) | 0.0547 (10) | 0.0079 (6) | 0.0127 (7) | −0.0027 (7) |
| C1A | 0.0226 (7) | 0.0267 (7) | 0.0274 (8) | 0.0066 (6) | 0.0109 (6) | 0.0108 (6) |
| C2A | 0.0348 (9) | 0.0271 (7) | 0.0290 (8) | 0.0113 (7) | 0.0162 (7) | 0.0115 (6) |
| C3A | 0.0383 (9) | 0.0254 (7) | 0.0253 (8) | −0.0012 (7) | 0.0126 (7) | 0.0063 (6) |
| C4A | 0.0247 (8) | 0.0376 (9) | 0.0286 (8) | 0.0005 (7) | 0.0082 (7) | 0.0080 (7) |
| C5A | 0.0220 (7) | 0.0341 (8) | 0.0304 (8) | 0.0084 (6) | 0.0099 (6) | 0.0093 (7) |
| C6A | 0.0206 (7) | 0.0264 (7) | 0.0235 (7) | 0.0067 (6) | 0.0104 (6) | 0.0082 (6) |
| C7A | 0.0184 (7) | 0.0269 (7) | 0.0242 (7) | 0.0089 (6) | 0.0104 (6) | 0.0096 (6) |
| C8A | 0.0200 (7) | 0.0291 (7) | 0.0280 (8) | 0.0102 (6) | 0.0126 (6) | 0.0100 (6) |
| C9A | 0.0223 (7) | 0.0258 (7) | 0.0231 (7) | 0.0114 (6) | 0.0113 (6) | 0.0092 (6) |
| C10A | 0.0246 (7) | 0.0249 (7) | 0.0232 (7) | 0.0105 (6) | 0.0122 (6) | 0.0099 (6) |
| C11A | 0.0274 (8) | 0.0240 (7) | 0.0254 (7) | 0.0104 (6) | 0.0138 (6) | 0.0086 (6) |
| C12A | 0.0268 (7) | 0.0253 (7) | 0.0215 (7) | 0.0125 (6) | 0.0116 (6) | 0.0097 (6) |
| C13A | 0.0264 (7) | 0.0261 (7) | 0.0213 (7) | 0.0132 (6) | 0.0114 (6) | 0.0083 (6) |
| C14A | 0.0268 (8) | 0.0263 (8) | 0.0400 (9) | 0.0114 (6) | 0.0116 (7) | −0.0005 (7) |
| C15A | 0.0231 (8) | 0.0308 (8) | 0.0427 (10) | 0.0090 (7) | 0.0099 (7) | −0.0020 (7) |
| C16A | 0.0273 (8) | 0.0290 (8) | 0.0263 (8) | 0.0155 (6) | 0.0089 (6) | 0.0058 (6) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C17A | 0.0347 (9) | 0.0233 (7) | 0.0306 (8) | 0.0135 (6) | 0.0152 (7) | 0.0079 (6) |
| C18A | 0.0294 (8) | 0.0246 (7) | 0.0333 (8) | 0.0096 (6) | 0.0155 (7) | 0.0106 (6) |
| C19A | 0.0248 (8) | 0.0251 (7) | 0.0344 (9) | 0.0091 (6) | 0.0059 (7) | 0.0001 (6) |
| C20A | 0.0208 (7) | 0.0236 (7) | 0.0251 (7) | 0.0104 (5) | 0.0124 (6) | 0.0104 (6) |
| C21A | 0.0240 (8) | 0.0363 (8) | 0.0241 (8) | 0.0106 (6) | 0.0099 (6) | 0.0071 (6) |
| C22A | 0.0216 (8) | 0.0509 (10) | 0.0327 (9) | 0.0183 (7) | 0.0119 (7) | 0.0153 (8) |
| C23A | 0.0320 (9) | 0.0443 (9) | 0.0317 (9) | 0.0253 (8) | 0.0206 (7) | 0.0170 (7) |
| C24A | 0.0334 (9) | 0.0349 (8) | 0.0245 (8) | 0.0169 (7) | 0.0136 (7) | 0.0092 (6) |
| C25A | 0.0219 (7) | 0.0289 (7) | 0.0248 (7) | 0.0108 (6) | 0.0091 (6) | 0.0100 (6) |
| Cl1B | 0.0461 (3) | 0.0250 (2) | 0.0414 (2) | 0.00970 (18) | 0.0042 (2) | −0.00243 (17) |
| S1B | 0.02187 (18) | 0.02330 (18) | 0.0385 (2) | 0.00744 (14) | 0.00972 (16) | 0.00539 (16) |
| F1B | 0.0310 (6) | 0.0397 (6) | 0.0831 (9) | 0.0154 (5) | 0.0356 (6) | 0.0135 (6) |
| N1B | 0.0209 (6) | 0.0196 (5) | 0.0251 (6) | 0.0076 (5) | 0.0106 (5) | 0.0067 (5) |
| N2B | 0.0247 (6) | 0.0195 (6) | 0.0252 (6) | 0.0084 (5) | 0.0119 (5) | 0.0064 (5) |
| N3B | 0.0237 (6) | 0.0209 (6) | 0.0221 (6) | 0.0089 (5) | 0.0104 (5) | 0.0060 (5) |
| N4B | 0.0287 (8) | 0.0238 (7) | 0.0653 (11) | 0.0086 (6) | 0.0160 (8) | 0.0040 (7) |
| C1B | 0.0272 (8) | 0.0258 (7) | 0.0251 (7) | 0.0105 (6) | 0.0100 (6) | 0.0101 (6) |
| C2B | 0.0352 (9) | 0.0292 (8) | 0.0226 (7) | 0.0165 (7) | 0.0093 (7) | 0.0074 (6) |
| C3B | 0.0327 (8) | 0.0202 (7) | 0.0257 (8) | 0.0121 (6) | 0.0019 (6) | 0.0036 (6) |
| C4B | 0.0230 (7) | 0.0252 (7) | 0.0340 (8) | 0.0068 (6) | 0.0064 (6) | 0.0098 (6) |
| C5B | 0.0216 (7) | 0.0255 (7) | 0.0268 (8) | 0.0095 (6) | 0.0085 (6) | 0.0076 (6) |
| C6B | 0.0211 (7) | 0.0235 (7) | 0.0215 (7) | 0.0103 (6) | 0.0059 (6) | 0.0076 (5) |
| C7B | 0.0215 (7) | 0.0224 (7) | 0.0223 (7) | 0.0080 (5) | 0.0097 (6) | 0.0083 (5) |
| C8B | 0.0210 (7) | 0.0242 (7) | 0.0256 (7) | 0.0083 (6) | 0.0104 (6) | 0.0076 (6) |
| C9B | 0.0239 (7) | 0.0224 (7) | 0.0231 (7) | 0.0101 (6) | 0.0107 (6) | 0.0087 (6) |
| C10B | 0.0241 (7) | 0.0201 (6) | 0.0232 (7) | 0.0076 (5) | 0.0099 (6) | 0.0081 (5) |
| C11B | 0.0267 (8) | 0.0208 (7) | 0.0306 (8) | 0.0088 (6) | 0.0102 (6) | 0.0044 (6) |
| C12B | 0.0252 (7) | 0.0213 (7) | 0.0221 (7) | 0.0095 (6) | 0.0105 (6) | 0.0075 (5) |
| C13B | 0.0247 (7) | 0.0229 (7) | 0.0188 (7) | 0.0090 (6) | 0.0095 (6) | 0.0055 (5) |
| C14B | 0.0271 (8) | 0.0199 (7) | 0.0281 (8) | 0.0084 (6) | 0.0105 (6) | 0.0045 (6) |
| C15B | 0.0251 (8) | 0.0231 (7) | 0.0364 (9) | 0.0071 (6) | 0.0120 (7) | 0.0058 (6) |
| C16B | 0.0251 (8) | 0.0244 (7) | 0.0280 (8) | 0.0112 (6) | 0.0109 (6) | 0.0053 (6) |
| C17B | 0.0304 (8) | 0.0194 (7) | 0.0280 (8) | 0.0091 (6) | 0.0124 (7) | 0.0033 (6) |
| C18B | 0.0250 (7) | 0.0218 (7) | 0.0269 (8) | 0.0062 (6) | 0.0105 (6) | 0.0044 (6) |
| C19B | 0.0275 (8) | 0.0212 (7) | 0.0408 (9) | 0.0061 (6) | 0.0122 (7) | 0.0035 (7) |
| C20B | 0.0183 (7) | 0.0229 (7) | 0.0244 (7) | 0.0073 (5) | 0.0093 (6) | 0.0063 (6) |
| C21B | 0.0261 (8) | 0.0227 (7) | 0.0408 (9) | 0.0075 (6) | 0.0168 (7) | 0.0119 (6) |
| C22B | 0.0294 (9) | 0.0306 (8) | 0.0555 (11) | 0.0076 (7) | 0.0270 (8) | 0.0154 (8) |
| C23B | 0.0203 (7) | 0.0299 (8) | 0.0472 (10) | 0.0095 (6) | 0.0176 (7) | 0.0067 (7) |
| C24B | 0.0258 (8) | 0.0259 (7) | 0.0416 (9) | 0.0126 (6) | 0.0128 (7) | 0.0111 (7) |
| C25B | 0.0236 (7) | 0.0268 (7) | 0.0321 (8) | 0.0100 (6) | 0.0132 (6) | 0.0126 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cl1A—C3A | 1.7401 (16) | Cl1B—C3B | 1.7428 (15) |
| S1A—C11A | 1.7044 (15) | S1B—C11B | 1.7055 (15) |
| S1A—C10A | 1.7325 (16) | S1B—C10B | 1.7312 (15) |
| F1A—C23A | 1.3617 (17) | F1B—C23B | 1.3647 (17) |

| | | | |
|---|---|---|---|
| N1A—N2A | 1.3622 (16) | N1B—N2B | 1.3570 (16) |
| N1A—C7A | 1.3761 (18) | N1B—C7B | 1.3749 (18) |
| N1A—C20A | 1.4273 (17) | N1B—C20B | 1.4314 (18) |
| N2A—C9A | 1.3377 (18) | N2B—C9B | 1.3411 (18) |
| N3A—C10A | 1.3063 (18) | N3B—C10B | 1.3124 (19) |
| N3A—C12A | 1.3879 (18) | N3B—C12B | 1.3895 (18) |
| N4A—C19A | 1.148 (2) | N4B—C19B | 1.148 (2) |
| C1A—C2A | 1.390 (2) | C1B—C2B | 1.390 (2) |
| C1A—C6A | 1.397 (2) | C1B—C6B | 1.398 (2) |
| C1A—H1AA | 0.9300 | C1B—H1BA | 0.9300 |
| C2A—C3A | 1.386 (2) | C2B—C3B | 1.384 (2) |
| C2A—H2AA | 0.9300 | C2B—H2BA | 0.9300 |
| C3A—C4A | 1.385 (2) | C3B—C4B | 1.387 (2) |
| C4A—C5A | 1.384 (2) | C4B—C5B | 1.388 (2) |
| C4A—H4AA | 0.9300 | C4B—H4BA | 0.9300 |
| C5A—C6A | 1.403 (2) | C5B—C6B | 1.400 (2) |
| C5A—H5AA | 0.9300 | C5B—H5BA | 0.9300 |
| C6A—C7A | 1.473 (2) | C6B—C7B | 1.474 (2) |
| C7A—C8A | 1.379 (2) | C7B—C8B | 1.3808 (19) |
| C8A—C9A | 1.402 (2) | C8B—C9B | 1.402 (2) |
| C8A—H8AA | 0.9300 | C8B—H8BA | 0.9300 |
| C9A—C10A | 1.459 (2) | C9B—C10B | 1.459 (2) |
| C11A—C12A | 1.372 (2) | C11B—C12B | 1.369 (2) |
| C11A—H11A | 0.9300 | C11B—H11B | 0.9300 |
| C12A—C13A | 1.471 (2) | C12B—C13B | 1.473 (2) |
| C13A—C14A | 1.396 (2) | C13B—C14B | 1.400 (2) |
| C13A—C18A | 1.401 (2) | C13B—C18B | 1.401 (2) |
| C14A—C15A | 1.384 (2) | C14B—C15B | 1.387 (2) |
| C14A—H14B | 0.9300 | C14B—H14A | 0.9300 |
| C15A—C16A | 1.396 (2) | C15B—C16B | 1.402 (2) |
| C15A—H15B | 0.9300 | C15B—H15A | 0.9300 |
| C16A—C17A | 1.398 (2) | C16B—C17B | 1.397 (2) |
| C16A—C19A | 1.444 (2) | C16B—C19B | 1.445 (2) |
| C17A—C18A | 1.381 (2) | C17B—C18B | 1.377 (2) |
| C17A—H17B | 0.9300 | C17B—H17A | 0.9300 |
| C18A—H18B | 0.9300 | C18B—H18A | 0.9300 |
| C20A—C25A | 1.385 (2) | C20B—C25B | 1.388 (2) |
| C20A—C21A | 1.385 (2) | C20B—C21B | 1.388 (2) |
| C21A—C22A | 1.389 (2) | C21B—C22B | 1.390 (2) |
| C21A—H21B | 0.9300 | C21B—H21A | 0.9300 |
| C22A—C23A | 1.370 (2) | C22B—C23B | 1.376 (2) |
| C22A—H22B | 0.9300 | C22B—H22A | 0.9300 |
| C23A—C24A | 1.377 (2) | C23B—C24B | 1.377 (2) |
| C24A—C25A | 1.386 (2) | C24B—C25B | 1.387 (2) |
| C24A—H24B | 0.9300 | C24B—H24A | 0.9300 |
| C25A—H25B | 0.9300 | C25B—H25A | 0.9300 |
| | | | |
| C11A—S1A—C10A | 89.00 (7) | C11B—S1B—C10B | 88.81 (7) |

| | | | |
|---|---|---|---|
| N2A—N1A—C7A | 112.26 (11) | N2B—N1B—C7B | 112.35 (11) |
| N2A—N1A—C20A | 117.81 (11) | N2B—N1B—C20B | 119.34 (12) |
| C7A—N1A—C20A | 129.66 (12) | C7B—N1B—C20B | 128.31 (12) |
| C9A—N2A—N1A | 104.36 (12) | C9B—N2B—N1B | 104.17 (12) |
| C10A—N3A—C12A | 110.04 (13) | C10B—N3B—C12B | 109.82 (12) |
| C2A—C1A—C6A | 120.19 (15) | C2B—C1B—C6B | 120.61 (14) |
| C2A—C1A—H1AA | 119.9 | C2B—C1B—H1BA | 119.7 |
| C6A—C1A—H1AA | 119.9 | C6B—C1B—H1BA | 119.7 |
| C3A—C2A—C1A | 119.69 (15) | C3B—C2B—C1B | 119.22 (15) |
| C3A—C2A—H2AA | 120.2 | C3B—C2B—H2BA | 120.4 |
| C1A—C2A—H2AA | 120.2 | C1B—C2B—H2BA | 120.4 |
| C4A—C3A—C2A | 121.18 (15) | C2B—C3B—C4B | 121.55 (14) |
| C4A—C3A—Cl1A | 119.05 (13) | C2B—C3B—Cl1B | 119.01 (13) |
| C2A—C3A—Cl1A | 119.75 (14) | C4B—C3B—Cl1B | 119.42 (13) |
| C5A—C4A—C3A | 118.95 (15) | C3B—C4B—C5B | 118.84 (15) |
| C5A—C4A—H4AA | 120.5 | C3B—C4B—H4BA | 120.6 |
| C3A—C4A—H4AA | 120.5 | C5B—C4B—H4BA | 120.6 |
| C4A—C5A—C6A | 121.13 (15) | C4B—C5B—C6B | 120.98 (14) |
| C4A—C5A—H5AA | 119.4 | C4B—C5B—H5BA | 119.5 |
| C6A—C5A—H5AA | 119.4 | C6B—C5B—H5BA | 119.5 |
| C1A—C6A—C5A | 118.80 (14) | C1B—C6B—C5B | 118.80 (13) |
| C1A—C6A—C7A | 123.26 (13) | C1B—C6B—C7B | 122.35 (13) |
| C5A—C6A—C7A | 117.93 (14) | C5B—C6B—C7B | 118.81 (13) |
| N1A—C7A—C8A | 105.87 (13) | N1B—C7B—C8B | 106.21 (12) |
| N1A—C7A—C6A | 124.12 (13) | N1B—C7B—C6B | 124.85 (13) |
| C8A—C7A—C6A | 130.00 (13) | C8B—C7B—C6B | 128.87 (13) |
| C7A—C8A—C9A | 105.62 (13) | C7B—C8B—C9B | 105.04 (13) |
| C7A—C8A—H8AA | 127.2 | C7B—C8B—H8BA | 127.5 |
| C9A—C8A—H8AA | 127.2 | C9B—C8B—H8BA | 127.5 |
| N2A—C9A—C8A | 111.89 (13) | N2B—C9B—C8B | 112.23 (13) |
| N2A—C9A—C10A | 118.99 (13) | N2B—C9B—C10B | 118.76 (13) |
| C8A—C9A—C10A | 129.10 (13) | C8B—C9B—C10B | 129.00 (14) |
| N3A—C10A—C9A | 123.79 (14) | N3B—C10B—C9B | 125.06 (13) |
| N3A—C10A—S1A | 115.43 (11) | N3B—C10B—S1B | 115.54 (11) |
| C9A—C10A—S1A | 120.78 (11) | C9B—C10B—S1B | 119.37 (11) |
| C12A—C11A—S1A | 110.82 (11) | C12B—C11B—S1B | 111.18 (11) |
| C12A—C11A—H11A | 124.6 | C12B—C11B—H11B | 124.4 |
| S1A—C11A—H11A | 124.6 | S1B—C11B—H11B | 124.4 |
| C11A—C12A—N3A | 114.71 (13) | C11B—C12B—N3B | 114.62 (13) |
| C11A—C12A—C13A | 126.63 (14) | C11B—C12B—C13B | 125.19 (13) |
| N3A—C12A—C13A | 118.64 (13) | N3B—C12B—C13B | 120.14 (13) |
| C14A—C13A—C18A | 118.52 (14) | C14B—C13B—C18B | 118.50 (13) |
| C14A—C13A—C12A | 120.22 (13) | C14B—C13B—C12B | 121.88 (13) |
| C18A—C13A—C12A | 121.24 (14) | C18B—C13B—C12B | 119.61 (13) |
| C15A—C14A—C13A | 121.12 (15) | C15B—C14B—C13B | 120.98 (14) |
| C15A—C14A—H14B | 119.4 | C15B—C14B—H14A | 119.5 |
| C13A—C14A—H14B | 119.4 | C13B—C14B—H14A | 119.5 |
| C14A—C15A—C16A | 119.65 (16) | C14B—C15B—C16B | 119.36 (14) |

| | | | |
|---|---|---|---|
| C14A—C15A—H15B | 120.2 | C14B—C15B—H15A | 120.3 |
| C16A—C15A—H15B | 120.2 | C16B—C15B—H15A | 120.3 |
| C15A—C16A—C17A | 119.99 (14) | C17B—C16B—C15B | 120.22 (14) |
| C15A—C16A—C19A | 119.77 (15) | C17B—C16B—C19B | 118.43 (13) |
| C17A—C16A—C19A | 120.17 (14) | C15B—C16B—C19B | 121.34 (14) |
| C18A—C17A—C16A | 119.70 (14) | C18B—C17B—C16B | 119.62 (14) |
| C18A—C17A—H17B | 120.2 | C18B—C17B—H17A | 120.2 |
| C16A—C17A—H17B | 120.2 | C16B—C17B—H17A | 120.2 |
| C17A—C18A—C13A | 121.01 (15) | C17B—C18B—C13B | 121.30 (14) |
| C17A—C18A—H18B | 119.5 | C17B—C18B—H18A | 119.3 |
| C13A—C18A—H18B | 119.5 | C13B—C18B—H18A | 119.3 |
| N4A—C19A—C16A | 176.7 (2) | N4B—C19B—C16B | 178.14 (17) |
| C25A—C20A—C21A | 120.93 (14) | C25B—C20B—C21B | 121.52 (13) |
| C25A—C20A—N1A | 120.26 (13) | C25B—C20B—N1B | 119.10 (13) |
| C21A—C20A—N1A | 118.80 (13) | C21B—C20B—N1B | 119.32 (13) |
| C20A—C21A—C22A | 119.68 (15) | C20B—C21B—C22B | 119.32 (14) |
| C20A—C21A—H21B | 120.2 | C20B—C21B—H21A | 120.3 |
| C22A—C21A—H21B | 120.2 | C22B—C21B—H21A | 120.3 |
| C23A—C22A—C21A | 118.22 (15) | C23B—C22B—C21B | 118.09 (15) |
| C23A—C22A—H22B | 120.9 | C23B—C22B—H22A | 121.0 |
| C21A—C22A—H22B | 120.9 | C21B—C22B—H22A | 121.0 |
| F1A—C23A—C22A | 118.52 (15) | F1B—C23B—C22B | 118.39 (15) |
| F1A—C23A—C24A | 118.24 (15) | F1B—C23B—C24B | 118.19 (14) |
| C22A—C23A—C24A | 123.24 (15) | C22B—C23B—C24B | 123.42 (14) |
| C23A—C24A—C25A | 118.27 (15) | C23B—C24B—C25B | 118.34 (14) |
| C23A—C24A—H24B | 120.9 | C23B—C24B—H24A | 120.8 |
| C25A—C24A—H24B | 120.9 | C25B—C24B—H24A | 120.8 |
| C20A—C25A—C24A | 119.63 (14) | C24B—C25B—C20B | 119.20 (14) |
| C20A—C25A—H25B | 120.2 | C24B—C25B—H25A | 120.4 |
| C24A—C25A—H25B | 120.2 | C20B—C25B—H25A | 120.4 |
| | | | |
| C7A—N1A—N2A—C9A | −0.46 (16) | C7B—N1B—N2B—C9B | 0.54 (16) |
| C20A—N1A—N2A—C9A | 174.20 (12) | C20B—N1B—N2B—C9B | −179.95 (12) |
| C6A—C1A—C2A—C3A | −0.9 (2) | C6B—C1B—C2B—C3B | 0.7 (2) |
| C1A—C2A—C3A—C4A | −1.4 (2) | C1B—C2B—C3B—C4B | 0.0 (2) |
| C1A—C2A—C3A—Cl1A | 176.82 (12) | C1B—C2B—C3B—Cl1B | −178.65 (12) |
| C2A—C3A—C4A—C5A | 2.3 (2) | C2B—C3B—C4B—C5B | −0.3 (2) |
| Cl1A—C3A—C4A—C5A | −175.97 (12) | Cl1B—C3B—C4B—C5B | 178.40 (12) |
| C3A—C4A—C5A—C6A | −0.9 (2) | C3B—C4B—C5B—C6B | −0.2 (2) |
| C2A—C1A—C6A—C5A | 2.3 (2) | C2B—C1B—C6B—C5B | −1.1 (2) |
| C2A—C1A—C6A—C7A | −178.81 (14) | C2B—C1B—C6B—C7B | −178.93 (14) |
| C4A—C5A—C6A—C1A | −1.4 (2) | C4B—C5B—C6B—C1B | 0.8 (2) |
| C4A—C5A—C6A—C7A | 179.62 (14) | C4B—C5B—C6B—C7B | 178.76 (14) |
| N2A—N1A—C7A—C8A | 0.16 (17) | N2B—N1B—C7B—C8B | −0.64 (16) |
| C20A—N1A—C7A—C8A | −173.70 (14) | C20B—N1B—C7B—C8B | 179.92 (13) |
| N2A—N1A—C7A—C6A | 179.59 (13) | N2B—N1B—C7B—C6B | 176.52 (13) |
| C20A—N1A—C7A—C6A | 5.7 (2) | C20B—N1B—C7B—C6B | −2.9 (2) |
| C1A—C6A—C7A—N1A | 37.1 (2) | C1B—C6B—C7B—N1B | −36.7 (2) |

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|---|---|---|---|
| C5A—C6A—C7A—N1A | −143.99 (15) | C5B—C6B—C7B—N1B | 145.41 (14) |
| C1A—C6A—C7A—C8A | −143.60 (17) | C1B—C6B—C7B—C8B | 139.76 (16) |
| C5A—C6A—C7A—C8A | 35.3 (2) | C5B—C6B—C7B—C8B | −38.1 (2) |
| N1A—C7A—C8A—C9A | 0.20 (16) | N1B—C7B—C8B—C9B | 0.44 (16) |
| C6A—C7A—C8A—C9A | −179.19 (15) | C6B—C7B—C8B—C9B | −176.56 (14) |
| N1A—N2A—C9A—C8A | 0.59 (17) | N1B—N2B—C9B—C8B | −0.24 (16) |
| N1A—N2A—C9A—C10A | −178.03 (12) | N1B—N2B—C9B—C10B | −179.58 (12) |
| C7A—C8A—C9A—N2A | −0.51 (18) | C7B—C8B—C9B—N2B | −0.13 (17) |
| C7A—C8A—C9A—C10A | 177.94 (15) | C7B—C8B—C9B—C10B | 179.12 (14) |
| C12A—N3A—C10A—C9A | −179.85 (13) | C12B—N3B—C10B—C9B | −176.26 (13) |
| C12A—N3A—C10A—S1A | −0.36 (16) | C12B—N3B—C10B—S1B | 1.59 (16) |
| N2A—C9A—C10A—N3A | 163.76 (14) | N2B—C9B—C10B—N3B | 170.87 (14) |
| C8A—C9A—C10A—N3A | −14.6 (3) | C8B—C9B—C10B—N3B | −8.3 (2) |
| N2A—C9A—C10A—S1A | −15.70 (19) | N2B—C9B—C10B—S1B | −6.90 (18) |
| C8A—C9A—C10A—S1A | 165.95 (13) | C8B—C9B—C10B—S1B | 173.89 (12) |
| C11A—S1A—C10A—N3A | 0.31 (12) | C11B—S1B—C10B—N3B | −1.16 (12) |
| C11A—S1A—C10A—C9A | 179.81 (13) | C11B—S1B—C10B—C9B | 176.82 (12) |
| C10A—S1A—C11A—C12A | −0.15 (12) | C10B—S1B—C11B—C12B | 0.34 (12) |
| S1A—C11A—C12A—N3A | −0.01 (17) | S1B—C11B—C12B—N3B | 0.48 (17) |
| S1A—C11A—C12A—C13A | 178.17 (12) | S1B—C11B—C12B—C13B | −176.84 (11) |
| C10A—N3A—C12A—C11A | 0.24 (18) | C10B—N3B—C12B—C11B | −1.32 (18) |
| C10A—N3A—C12A—C13A | −178.10 (13) | C10B—N3B—C12B—C13B | 176.15 (12) |
| C11A—C12A—C13A—C14A | −177.63 (16) | C11B—C12B—C13B—C14B | −163.03 (15) |
| N3A—C12A—C13A—C14A | 0.5 (2) | N3B—C12B—C13B—C14B | 19.8 (2) |
| C11A—C12A—C13A—C18A | 0.8 (2) | C11B—C12B—C13B—C18B | 17.9 (2) |
| N3A—C12A—C13A—C18A | 178.91 (14) | N3B—C12B—C13B—C18B | −159.31 (13) |
| C18A—C13A—C14A—C15A | −0.8 (3) | C18B—C13B—C14B—C15B | −1.2 (2) |
| C12A—C13A—C14A—C15A | 177.70 (16) | C12B—C13B—C14B—C15B | 179.68 (14) |
| C13A—C14A—C15A—C16A | −0.5 (3) | C13B—C14B—C15B—C16B | 0.0 (2) |
| C14A—C15A—C16A—C17A | 1.3 (3) | C14B—C15B—C16B—C17B | 0.8 (2) |
| C14A—C15A—C16A—C19A | −175.72 (17) | C14B—C15B—C16B—C19B | −179.99 (15) |
| C15A—C16A—C17A—C18A | −0.8 (2) | C15B—C16B—C17B—C18B | −0.5 (2) |
| C19A—C16A—C17A—C18A | 176.16 (15) | C19B—C16B—C17B—C18B | −179.70 (15) |
| C16A—C17A—C18A—C13A | −0.4 (2) | C16B—C17B—C18B—C13B | −0.7 (2) |
| C14A—C13A—C18A—C17A | 1.2 (2) | C14B—C13B—C18B—C17B | 1.6 (2) |
| C12A—C13A—C18A—C17A | −177.22 (14) | C12B—C13B—C18B—C17B | −179.31 (14) |
| N2A—N1A—C20A—C25A | −124.58 (15) | N2B—N1B—C20B—C25B | 129.87 (15) |
| C7A—N1A—C20A—C25A | 49.0 (2) | C7B—N1B—C20B—C25B | −50.7 (2) |
| N2A—N1A—C20A—C21A | 54.44 (18) | N2B—N1B—C20B—C21B | −52.93 (19) |
| C7A—N1A—C20A—C21A | −131.98 (16) | C7B—N1B—C20B—C21B | 126.48 (16) |
| C25A—C20A—C21A—C22A | −1.0 (2) | C25B—C20B—C21B—C22B | 1.9 (3) |
| N1A—C20A—C21A—C22A | 179.96 (14) | N1B—C20B—C21B—C22B | −175.22 (15) |
| C20A—C21A—C22A—C23A | 0.2 (3) | C20B—C21B—C22B—C23B | 1.3 (3) |
| C21A—C22A—C23A—F1A | −179.16 (15) | C21B—C22B—C23B—F1B | 176.88 (16) |
| C21A—C22A—C23A—C24A | 0.2 (3) | C21B—C22B—C23B—C24B | −3.3 (3) |
| F1A—C23A—C24A—C25A | 179.68 (14) | F1B—C23B—C24B—C25B | −178.21 (15) |
| C22A—C23A—C24A—C25A | 0.3 (3) | C22B—C23B—C24B—C25B | 2.0 (3) |
| C21A—C20A—C25A—C24A | 1.6 (2) | C23B—C24B—C25B—C20B | 1.3 (2) |

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|---|---|---|---|
| N1A—C20A—C25A—C24A | −179.45 (13) | C21B—C20B—C25B—C24B | −3.3 (2) |
| C23A—C24A—C25A—C20A | −1.2 (2) | N1B—C20B—C25B—C24B | 173.87 (14) |

*Hydrogen-bond geometry (Å, º)*

Cg1 and Cg2 are the centroids of the C1A–C6A and C1B–C6B rings, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C5*A*—H5*AA*···F1*A*$^{i}$ | 0.93 | 2.39 | 3.149 (2) | 138 |
| C8*B*—H8*BA*···F1*B*$^{i}$ | 0.93 | 2.42 | 3.283 (2) | 154 |
| C17*B*—H17*A*···N4*A*$^{ii}$ | 0.93 | 2.54 | 3.419 (2) | 159 |
| C17*A*—H17*B*···N4*B*$^{ii}$ | 0.93 | 2.58 | 3.453 (2) | 156 |
| C25*B*—H25*A*···N2*A*$^{iii}$ | 0.93 | 2.53 | 3.457 (2) | 175 |
| C24*A*—H24*B*···*Cg*1$^{iv}$ | 0.93 | 2.96 | 3.7811 (18) | 148 |
| C21*B*—H21*A*···*Cg*2$^{v}$ | 0.93 | 2.97 | 3.6423 (19) | 131 |

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