Crystal structure and Hirshfeld surface analysis of 5-acetyl-3-amino-6-methyl-N-phenyl-4-[(E)-2-phenylethenyl]thieno[2,3-b]pyridine-2-carboxamide

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The asymmetric unit of the title compound, C_{25}H_{21}N_{3}O_{2}S, comprises four molecules. Their conformations differ primarily in the orientations of the styryl and the N-phenylcarboxamido groups. In the crystal, intermolecular N—H⋯N, C—H⋯O and C—H⋯S hydrogen-bonding contacts as well as C—H⋯π(ring) interactions lead to the formation of a layer structure parallel to (010). Hirshfeld surface analysis revealed that H⋯H interactions represent the main contributions to the crystal packing.

1. Chemical context

Thienopyridine derivatives are well known to possess various functional and medicinal properties with general applications as synthetic building blocks or as pharmaceuticals (Litvinov et al., 2005; Dotsenko et al., 2020; Bakhite, 2003; Al-Waleedy et al., 2020; Abuelhassan et al., 2021). Many thienopyridines are reported to show anticancer (Zeng et al., 2010), antiparasitic (Bernardino et al., 2006), insecticidal (El-Dean et al., 2019), antimicrobial (Abdel-Rahman et al., 2003; Eldin, 1999) and antidiabetic (Bahekar et al., 2007) activities. Encouraged by the above facts, we report in this communication the synthesis and crystal structure determination of the title compound, C_{25}H_{21}N_{3}O_{2}S (I).

2. Structural commentary

The asymmetric unit of (I) contains four molecules (Fig. 1) of which one (molecule I) is represented in an ORTEP-style plot.
in Fig. 2. The conformational differences between molecules I, II, III and IV are highlighted in the overlay diagram shown in Fig. 3. The maximum r.m.s. deviation of the overlay between molecules I, II, III and IV is 0.498 Å. The conformations of the four molecules differ primarily in the varying orientations of the styryl and the N-phenylcarboxamido groups, as indicated by the torsion and dihedral angles collated in Tables 1 and 2. The orientations of the latter substituents are partially deter-

Table 1
Selected torsion angles (°).

| Molecule I   | Molecule III |
|--------------|--------------|
| C4—C3—C9—C10 | 126.8 (2)    |
| C9—C10—C11—C12 | 162.2 (2)    |
| C19—N3—C20—C21 | −9.9 (3)     |
| C29—C34—C35 | −51.8 (3)    |
| C34—C35—C36—C41 | 178.4 (2)    |
| C44—N6—C45—C50 | −23.3 (3)    |

Table 2
Dihedral angles (°).

| Planes | Angle |
|--------|-------|
| Molecule I |       |
| N1/C1—C5 vs C4/C5/S1/C17/C18 | 2.18 (8) |
| N1/C1—C5 vs C10—C16 | 70.47 (5) |
| N1/C1—C5 vs C20—C25 | 12.78 (8) |
| Molecule II |       |
| N4/C26—C30 vs C29/C30/S2/C43/C42 | 4.0 (1) |
| N4/C26—C30 vs C36—C41 | 47.01 (5) |
| N4/C26—C30 vs C45—C50 | 27.4 (1) |
| Molecule III |       |
| N7/C51—C55 vs C54/C55/S3/C68/C67 | 3.20 (8) |
| N7/C51—C55 vs C61—C66 | 48.96 (6) |
| N7/C51—C55 vs C70—C75 | 35.64 (8) |
| Molecule IV |       |
| N10/C76—C80 vs C80/S4/C93/C92 | 2.4 (1) |
| N10/C76—C80 vs C95—C100 | 32.11 (8) |
| N10/C76—C80 vs C96—C91 | 77.15 (6) |

in the crystal, various hydrogen-bonding interactions are found (Table 3). The strongest stem from interactions between the amide NH group and the pyridine N atom of a neigh-

Figure 1
The four molecules (I, II, III and IV) in the asymmetric unit of (I).

Figure 2
Molecule I with displacement ellipsoids for the non-hydrogen atoms drawn at the 30% probability level. The intramolecular N—H···O hydrogen bond is depicted by a dashed line.

Figure 3
Overlay image of the four molecules (I, II, III and IV) in the asymmetric unit of the title compound.

3. Supramolecular features

In the crystal, various hydrogen-bonding interactions are found (Table 3). The strongest stem from interactions between the amide NH group and the pyridine N atom of a neigh-

Figure 1
The four molecules (I, II, III and IV) in the asymmetric unit of (I).

Figure 2
Molecule I with displacement ellipsoids for the non-hydrogen atoms drawn at the 30% probability level. The intramolecular N—H···O hydrogen bond is depicted by a dashed line.
the packing. Together with three sets of C—H⋯π(ring) interactions, supramolecular layers parallel to the ac plane with a width corresponding to b/2 are formed (Figs. 4 and 5).

4. Hirshfeld surface analysis

For the four molecules I, II, III and IV, intermolecular interactions (Table 4) were quantified using Hirshfeld surface analysis and the associated two-dimensional fingerprint plots generated. The calculations and visualization were carried out using Crystal Explorer 17.5 (Turner et al., 2017). Fig. 6 shows the Hirshfeld surface of the four molecules in (I) mapped over \(d_{\text{norm}}\) in a fixed colour scale of −0.3297 (red) to +1.5167 (blue) a.u. for molecule I, −0.3246 (red) to +1.4683 (blue) a.u. for molecule II, −0.3890 (red) to +2.0338 (blue) a.u. for molecule III, and −0.3870 (red) to +1.8555 (blue) a.u. for molecule IV. The red spots on the Hirshfeld surface are indicative of contacts shorter than van der Waals separations and represent N—H⋯N, N—H⋯O, C—H⋯O and C—H⋯S contacts. Fig. 7 displays the full two-dimensional fingerprint plot and those delineated into the major contacts of H⋯H interactions (46.5\% contribution for I; 47.0\% for II; 44.7\% for III; 45.5\% for IV) are the major factor in the crystal packing with C—H⋯H—C (22.7\% for I; 27.9\% for II; 28.1\% for III; 20.2\% for IV) and O⋯H⋯O (9.7\% for I; 8.9\% for II; 11.3\% for III; 12.6\% for IV) interactions representing the next highest

| Contact | Distance | Symmetry operation |
|---------|----------|--------------------|
| H3A···N4 | 2.31 | \(x, y - \frac{1}{2}, z + \frac{1}{2}\) |
| O1···H40 | 2.64 | \(x, y + \frac{1}{2}, z + \frac{1}{2}\) |
| H13···H8C | 2.38 | \(-x, 1 - y, 1 - z\) |
| H21···H97 | 2.33 | \(-x, y, \frac{1}{2} - z\) |
| N1···H12A | 2.30 | \(-x, -y, -z\) |
| H2B···O7 | 2.62 | \(x, y + \frac{1}{2}, z + \frac{1}{2}\) |
| H2A···H60 | 2.55 | \(x, y, z\) |
| C5···H22 | 3.03 | \(-x, 1 - y, 1 - z\) |
| C8···H47 | 3.09 | \(-x, -y, -z\) |
| H15···O3 | 2.71 | \(x, y, z\) |
| H24···H83B | 2.58 | \(-x, \frac{1}{2} + y, \frac{1}{2} - z\) |
| H6C···H87 | 2.42 | \(-x, \frac{1}{2} + y, \frac{1}{2} - z\) |
| H13···C48 | 3.06 | \(x, y, z\) |
| H24···C50 | 3.07 | \(-x, \frac{1}{2} + y, \frac{1}{2} - z\) |
| H6D···N7 | 2.38 | \(-x, \frac{1}{2} + y, \frac{1}{2} - z\) |
| O3···H8E | 2.55 | \((-x, -y, -z)\) |
| H33C···O8 | 2.47 | \((-x, -y, -z)\) |
| H5A···H56C | 2.40 | \((-x, -y, -z)\) |
| H49···C28 | 3.06 | \((-x, -y, -z)\) |
| H31A···H89 | 2.33 | \((-x, -y, -z)\) |
| H33C···H74 | 2.42 | \((-x, -y, -z)\) |
| H38···H81A | 2.44 | \((-x, -y, -z)\) |
| H47···C71 | 2.95 | \((-x, -y, -z)\) |
| H9A···N10 | 2.22 | \((-x, -y, -z)\) |
| O5···H90 | 2.69 | \((-x, -y, -z)\) |
| O5···H97 | 2.75 | \((-x, -y, -z)\) |
| H64···O5 | 2.72 | \((-x, -y, -z)\) |
| C53···H72 | 3.03 | \((-x, -y, -z)\) |
| H62···O7 | 2.64 | \((-x, -y, -z)\) |
| H65···C98 | 2.89 | \((-x, -y, -z)\) |
| H99···C76 | 2.90 | \((-x, -y, -z)\) |
contributions. The percentage contributions of other weak interactions are listed in Table 5.

The fact that the same interactions result in different contributions to the Hirshfeld surface for molecules I, II, III and IV can be attributed to the different environments of each molecule in the crystalline state.

Table 5

| Contact            | Molecule I | Molecule II | Molecule III | Molecule IV |
|--------------------|------------|-------------|--------------|-------------|
| H···H              | 46.5       | 47.0        | 44.7         | 45.5        |
| C···H/H···C        | 22.7       | 27.9        | 28.1         | 20.2        |
| O···H/H···O        | 9.7        | 8.9         | 11.3         | 12.6        |
| N···H/H···N        | 5.1        | 5.5         | 5.0          | 6.5         |
| S···H/H···S        | 3.2        | 2.9         | 3.3          | 3.4         |
| O···C/C···O        | 2.5        | 1.4         | 1.2          | 0.4         |
| S···N/N···S        | 1.5        | 1.5         | 1.1          | 1.1         |
| S···C/C···S        | 1.3        | 0.7         | 1.1          | 1.6         |
| S···S              | 1.3        | 1.2         | 1.2          | 1.0         |
| N···C/C···N        | 1.1        | 0.8         | 1.0          | 1.6         |
| O···O/H/H·O        | 0.2        | 0.0         | 0.1          | 0.0         |
| S···N/N···S        | 1.5        | 1.5         | 1.1          | 1.1         |
| S···C/C···S        | 1.3        | 0.7         | 1.1          | 1.6         |
| N···C/C···N        | 1.1        | 0.8         | 1.0          | 1.6         |
| N···N              | 1.1        | 0.8         | 1.0          | 1.6         |
| S···S              | 1.3        | 0.7         | 1.1          | 1.6         |
| N···C/C···N        | 1.1        | 0.8         | 1.0          | 1.6         |
| N···N              | 1.1        | 0.8         | 1.0          | 1.6         |

5. Database survey

A search of the Cambridge Structural Database (CSD Version 5.41, update of November 2019; Groom et al., 2016) for the thieno[2,3-b]pyridine moiety yielded ten structures closely related to the title compound: ethyl 3-amino-2-carbamoyl-4-(4-methoxyphenyl)-6-methylthieno-[2,3-b]pyridine-5-carboxylate dimethyl sulfoxide solvate (AWETIH; Bakhite et al., 2016a), ethyl 3-amino-4-(4-chlorophenyl)-2-[[4-methoxyphenyl]carbamoyl]-6-phenylthieno-

thieno[2,3-b]pyridine-2,5-dicarboxylate (MUZXOW; Mague et al., 2016b), 4-[[3-fluorophenyl]amino]thieno[2,3-b]pyridine-5-carboxylic acid (XEBPIF; Pinheiro et al., 2012), ethyl 3-amino-2-carbamoyl-4-(4-methoxyphenyl)-6-methylthieno-[2,3-b]pyridine-5-carboxylate dimethyl sulfoxide solvate (AWETIH; Bakhite et al., 2016a), ethyl 3-amino-4-(4-chlorophenyl)-2-[[4-methoxyphenyl]carbamoyl]-6-phenylthieno-

Figure 6

A view of the three-dimensional Hirshfeld surface for the four molecules (I, II, III and IV) in the asymmetric unit of the title compound, plotted over (a) \( d_{	ext{norm}} \) and (b) shape-index.

Figure 7

A view of the two-dimensional fingerprint plots for the four molecules (I, II, III and IV) in the asymmetric unit of the title compound, showing (a) all interactions, and delineated into (b) H···H, (c) C···H/H···C and (d) O···H/H···O interactions. The \( d_e \) and \( d_i \) values are the closest internal and external distances (in Å) from given points on the Hirshfeld surface.
[2,3-b]pyridine-5-carboxylate (ULAROQ; Bakhite et al., 2016b), ethyl 3-(4-methylbenzenesulfonylamido)thieno[2,3-b]pyridine-2-carboxylate (GOLDUH; Zhang et al., 2009), ethyl 3-aminothieno[2,3-b]pyridine-2-carboxylate (QOLPEN; Zheng et al., 2009), 4-(4-bromophenyl)-2,5-bis(ethoxycarbonyl)-6-methylthieno[2,3-b]pyridine (WUVZES; Novoa de Armas et al., 2003), 5-acetyl-3-amino-4-(4-methoxyphenyl)-6-methylthieno[2,3-b]pyridine-2-carbonitrile (NEQUSA; Mohamed et al., 2017) and 2-amino-6-benzyl-3-(ethoxycarbonyl)-4,5,6,7-tetrahydrothieno[2,3-c]pyridin-6-ium (hydrogen bis(4-methoxyphenyl)diphosphonate) (RUTRUV; Mague et al., 2015).

In the crystal of TACXED, mutual N–H⋯O hydrogen bonds form dimers, which are then associated into chains parallel to the c axis through O⋯H⋯N hydrogen bonds involving the solvent water molecule. In the crystal of MUZXOW, the bicyclic core of the compound is slightly folded [1.9 (1)°], while pairwise intermolecular N–H⋯O hydrogen bonding forms dimers across centres of symmetry. In the crystal of XEBPIF, an intramolecular N–H⋯O(carbonyl) hydrogen bond closes an S(6) ring. Supramolecular chains along [010] mediated by O⋯H⋯N(pyridine) hydrogen bonds form in the crystal. A three-dimensional network is completed by π⋯π interactions occurring between the benzenoid ring and the two rings of the thieno[2,3-b]pyridine unit. In the crystal of AWETIH, molecules are linked by pairs of N–H⋯O hydrogen bonds, forming inversion dimers with an R21(8) ring motif. Within the dimers, which stack along the a-axis direction, there is a weak π⋯π interaction involving inversion-related thiophene rings. In the crystal of ULAROQ, the conformation of the title molecule is partially determined by an intramolecular N–H⋯O hydrogen bond, forming an S(6) loop, and an N⋯H⋯O π interaction involving the centroid of the 4-chlorophenyl ring. In the crystal, molecules are linked by pairs of N–H⋯O hydrogen bonds, forming inversion dimers with an R21(20) ring motif. In the crystal of GOLDUH, the amino and carbonyl groups are nearly coplanar with the heterocyclic ring system. There are two N–H⋯O hydrogen-bonding interactions involving the same N–H donor set and two different acceptors, one in an intramolecular bond helping to fix the molecular conformation and the other defining a dimeric structure around the symmetry centre at (0, 1/2, 1/2).

The crystal structure is stabilized by intramolecular and intramolecular C–H⋯O hydrogen bonds. The asymmetric unit of NEQUSA likewise comprises two molecules, which differ primarily in the orientations of the acetyl and p-anisyl substituents. In the crystal, N⋯H⋯O hydrogen bonds form chains extending parallel to (110). The asymmetric unit of the molecular salt RUTRUV comprises two cations and two anions. Each cation features an intramolecular N–H⋯O hydrogen bond, which closes an S(6) ring; in each case the hydropyridine ring adopts a half-chair conformation. In the crystal, O⋯H⋯O and N⋯H⋯O hydrogen bonds link the components into [100] chains.

### Table 6

**Experimental details.**

| Crystal data | Chemical formula | C25H21N3O2S |
|--------------|------------------|---------------|
| Cell type    | M<sub>r</sub>     | 427.51        |
| System, space | Monoclinic, P2<sub>1</sub>/n |               |
| Temperature (K) | 150              |               |
| a, b, c (Å)  | 182782 (5), 191455 (6), 246978 (7) | |
| β (°)        | 96.323 (1)       |               |
| V (Å³)       | 8903.3 (4)       |               |
| Z             | 16               |               |
| Radiation type | Cu Kα             |               |
| μ (mm<sup>-1</sup>) | 1.56            |               |
| Crystal size (mm) | 0.43 x 0.35 x 0.13 | |

### Data collection

- **Diffractometer**: Bruker D8 VENTURE PHOTON 100 CMOS
- **Absorption correction**: Multi-scan (SADABS; Krause et al., 2015)
- **Max. T<sub>max</sub>**: 0.73, 0.82
- **No. of measured, independent and observed [I > 2σ(I)] reflections**: 65284, 17176, 14297
- **R<sub>int</sub>**: 0.038
- **(sin θ/λ)<sub>max</sub> (Å<sup>-1</sup>)**: 0.626
- **Refinement**: R[F<sup>2</sup> > 2σ(F<sup>2</sup>)], wR(F<sup>2</sup>), S 0.043, 0.114, 1.04
- **No. of reflections**: 17176
- **No. of parameters**: 1126
- **H-atom treatment**: H-atom parameters constrained
- **Δρ<sub>max</sub>, Δρ<sub>min</sub> (e Å<sup>-3</sup>)**: 0.68, −0.39

### Computer programs

- APEX3 and SAINT (Bruker, 2016), SHELXT (Sheeldrick, 2015a), SHELXL (Sheldrick, 2015b), DIAMOND (Brandenburg & Putz, 2012), OLEX2 (Dolomanov et al., 2009) and pubCIF (Westrip, 2010).

Numerous C–H⋯O interactions cross-link the chains into a three-dimensional network.

### 6. Synthesis and crystallization

To a suspension of 5-acetyl-3-cyano-1,2-dihydro-6-methyl-4-styryl-2-thioxopyridine (2.94 g, 10 mmol), N-phenyl-2-chloroacetamide (1.70 g, 10 mmol) in an ethanol solution (60 ml) was added, together with sodium ethoxide (22 mmol, 0.51 g sodium dissolved in 30 ml absolute ethanol). The resulting mixture was refluxed for 10 minutes. The solid that precipitated after cooling was collected and recrystallized from ethanol to give the title compound in the form of yellow crystals, yield 92%; m.p. 481–483 K. IR (cm<sup>-1</sup>): 3452, 3292, 3220 (NH<sub>2</sub>, NH), 3027 (C–H, aromatic), 1701 (C==O, acetyl) and 1633 (C==O, anilide).<sup>1</sup>H NMR: δ 9.59 (s, 1H, NH), 7.85–7.88 (d, J = 15 Hz, 1H, CH=CH), 7.07–7.69 (m, 10H, Ar–H), 6.79 (s, 2H, NH2), 6.71–6.74 (d, J = 15 Hz, 1H, C==CH), 2.52 (s, 3H, COCH<sub>3</sub>), δ 14.2 (s, 3H, CH<sub>3</sub> attached to pyridine ring).<sup>13</sup>C NMR: δ 205.61, 164.34, 158.93, 154.69, 148.61, 140.86, 139.61 (CH of CH==CH), 139.18, 136.00, 133.67, 129.59 (CH), 129.30 (CH), 128.89 (CH), 127.85 (CH), 124.12 (CH), 122.21 (CH of CH==CH), 122.02 (CH), 121.84 (CH), 121.85, 121.25, 98.87, 32.87 (CH<sub>3</sub> of acetyl group), 23.27 (CH<sub>3</sub> attached to pyridine ring). MS: m/z 427.14 (M<sup>+</sup> 100%). Analysis calculated for C<sub>25</sub>H<sub>21</sub>N<sub>3</sub>O<sub>2</sub>S (427.13): C 70.24, H 4.95, N 9.84%. Found: C 70.51, H 4.85, N 9.90%.

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7. Refinement details

Crystal data, data collection and structure refinement details are summarized in Table 6. H atoms attached to carbon were placed in calculated positions (C–H = 0.95–0.98 Å) while those attached to nitrogen were derived from a difference-Fourier map and their parameters adjusted to give N–H = 0.91 Å. All H atoms were included as riding contributions with isotropic displacement parameters 1.2–1.5 times those of the attached atoms.

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Crystal structure and Hirshfeld surface analysis of 5-acetyl-3-amino-6-methyl-N-phenyl-4-[(E)-2-phenylethenyl]thieno[2,3-b]pyridine-2-carboxamide

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Computing details

Data collection: APEX3 (Bruker, 2016); cell refinement: SAINT (Bruker, 2016); data reduction: SAINT (Bruker, 2016); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: SHELXL (Sheldrick, 2015b); molecular graphics: DIAMOND (Brandenburg & Putz, 2012), OLEX2 (Dolomanov et al., 2009); software used to prepare material for publication: publCIF (Westrip, 2010).

5-Acetyl-3-amino-6-methyl-N-phenyl-4-[(E)-2-phenylethenyl]thieno[2,3-b]pyridine-2-carboxamide

Crystal data

C₂₅H₂₁N₃O₂S  
Mr = 427.51  
Monoclinic, P2₁/n  
a = 18.2782 (5) Å  
b = 19.1455 (6) Å  
c = 24.6978 (7) Å  
β = 96.323 (1)°  
V = 8590.3 (4) Å³  
Z = 16 

Cu Kα radiation, λ = 1.54178 Å  
Cell parameters from 9118 reflections  
θ = 4.3–74.6°  
µ = 1.56 mm⁻¹  
T = 150 K  
Block, yellow  
0.43 × 0.35 × 0.13 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer  
Radiation source: INCOATEC μS micro-focus source  
Mirror monochromator  
Detector resolution: 10.4167 pixels mm⁻¹  
ω scans  
(SADABS; Krause et al., 2015)  

65284 measured reflections  
17176 independent reflections  
14297 reflections with I > 2σ(I)  
R(int) = 0.038  
θ(max) = 74.7°, θ(min) = 2.9°  
h = −22→22  
k = −23→22  
l = −29→30

Refinement

Refinement on F²  
Least-squares matrix: full  
R[F²] = 0.043  
wR(F²) = 0.114  
S = 1.04  
17176 reflections  
1126 parameters  
0 restraints

Primary atom site location: dual  
Secondary atom site location: difference Fourier map  
Hydrogen site location: mixed  
H-atom parameters constrained  

w = 1/[σ(Fo)² + (0.0485P)² + 4.7725P]  
where P = (Fo² + 2Fc²)/3  
(Δ/σ)max = 0.001

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$\Delta \rho_{\text{max}} = 0.68 \text{ e Å}^{-3}$

$\Delta \rho_{\text{min}} = -0.39 \text{ e Å}^{-3}$

Extinction correction: $SHELXL$ (Sheldrick, 2015b), $F^2 = kF^2[1 + 0.001xF^2]^3 \sin(2\theta)^{-1}$

Extinction coefficient: 0.00063 (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.

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. H-atoms attached to carbon were placed in calculated positions (C—H = 0.95 - 0.98 Å) while those attached to nitrogen were placed in locations derived from a difference map and their parameters adjusted to give N—H = 0.91 Å. All were included as riding contributions with isotropic displacement parameters 1.2 - 1.5 times those of the attached atoms.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\AA^2$)

| Atom | x     | y     | z     | Uiso*/$U_{eq}$ |
|------|-------|-------|-------|----------------|
| S1   | 0.62520 (3) | 0.30624 (2) | 0.17394 (2) | 0.03185 (10) |
| O1   | 0.55039 (8)  | 0.58307 (7)  | 0.31695 (6)  | 0.0421 (3)   |
| O2   | 0.64768 (8)  | 0.14490 (7)  | 0.27516 (5)  | 0.0406 (3)   |
| N1   | 0.58071 (8)  | 0.43773 (8)  | 0.18463 (6)  | 0.0300 (3)   |
| N2   | 0.59334 (9)  | 0.25628 (8)  | 0.32483 (6)  | 0.0324 (3)   |
| H2A  | 0.615181     | 0.213520     | 0.327535     | 0.039*       |
| H2B  | 0.600892     | 0.286081     | 0.353598     | 0.039*       |
| N3   | 0.67707 (8)  | 0.15460 (8)  | 0.18797 (6)  | 0.0320 (3)   |
| H3A  | 0.675877     | 0.183762     | 0.158792     | 0.038*       |
| C1   | 0.55522 (10) | 0.48828 (9)  | 0.21497 (7)  | 0.0308 (4)   |
| C2   | 0.53820 (10) | 0.47654 (9)  | 0.26873 (7)  | 0.0300 (4)   |
| C3   | 0.54733 (9)  | 0.41048 (9)  | 0.29249 (7)  | 0.0281 (3)   |
| C4   | 0.57713 (9)  | 0.35781 (9)  | 0.26157 (7)  | 0.0264 (3)   |
| C5   | 0.59141 (9)  | 0.37510 (9)  | 0.20844 (7)  | 0.0279 (3)   |
| C6   | 0.54387 (12) | 0.55831 (10) | 0.18774 (8)  | 0.0416 (4)   |
| H6A  | 0.492551     | 0.572890     | 0.188234     | 0.062*       |
| H6B  | 0.555166     | 0.554896     | 0.149948     | 0.062*       |
| H6C  | 0.576490     | 0.592769     | 0.207279     | 0.062*       |
| C7   | 0.50914 (11) | 0.53688 (10) | 0.29932 (7)  | 0.0330 (4)   |
| C8   | 0.42847 (11) | 0.53794 (11) | 0.30383 (9)  | 0.0414 (4)   |
| H8A  | 0.412776     | 0.491869     | 0.315429     | 0.062*       |
| H8B  | 0.401883     | 0.549543     | 0.268329     | 0.062*       |
| H8C  | 0.417730     | 0.573094     | 0.330690     | 0.062*       |
| C9   | 0.52653 (10) | 0.39531 (10) | 0.34737 (7)  | 0.0304 (4)   |
| H9   | 0.494318     | 0.357032     | 0.350899     | 0.037*       |
| C10  | 0.54946 (10) | 0.43121 (10) | 0.39249 (7)  | 0.0314 (4)   |
| H10  | 0.580706     | 0.470164     | 0.388737     | 0.038*       |
| C11  | 0.53033 (10) | 0.41539 (10) | 0.44731 (7)  | 0.0324 (4)   |
| C12  | 0.57324 (12) | 0.44375 (11) | 0.49233 (8)  | 0.0388 (4)   |
| Atom | x      | y        | z        | U(eq)     |
|------|--------|----------|----------|-----------|
| C12  | 0.613478 | 0.473367 | 0.486868 | 0.047*    |
| C13  | 0.55781 (14) | 0.42920 (12) | 0.54475 (8) | 0.0476 (5) |
| H13  | 0.587936 | 0.448134 | 0.575009 | 0.057*    |
| C14  | 0.49904 (15) | 0.38746 (12) | 0.55313 (8) | 0.0509 (6) |
| H14  | 0.488555 | 0.377599 | 0.589171 | 0.061*    |
| C15  | 0.45492 (14) | 0.35963 (12) | 0.50907 (9) | 0.0490 (5) |
| H15  | 0.413865 | 0.331271 | 0.514885 | 0.059*    |
| C16  | 0.47095 (12) | 0.37335 (11) | 0.45647 (8) | 0.0391 (4) |
| H16  | 0.440982 | 0.353784 | 0.426397 | 0.047*    |
| C17  | 0.59831 (9) | 0.28651 (9) | 0.27486 (7) | 0.0269 (3) |
| C18  | 0.62344 (9) | 0.25232 (9) | 0.23108 (7) | 0.0292 (4) |
| C19  | 0.64993 (9) | 0.18031 (10) | 0.23342 (7) | 0.0307 (4) |
| C20  | 0.70776 (10) | 0.08771 (10) | 0.18143 (7) | 0.0314 (4) |
| C21  | 0.72491 (11) | 0.04053 (11) | 0.22391 (8) | 0.0399 (4) |
| H21  | 0.715616 | 0.052318 | 0.259885 | 0.048*    |
| C22  | 0.75559 (12) | -0.02373 (11) | 0.21350 (9) | 0.0426 (5) |
| H22  | 0.767168 | -0.055687 | 0.242608 | 0.051*    |
| C23  | 0.76955 (12) | -0.04196 (11) | 0.16166 (9) | 0.0442 (5) |
| H23  | 0.790212 | -0.086241 | 0.154953 | 0.053*    |
| C24  | 0.75326 (14) | 0.00458 (13) | 0.11987 (9) | 0.0527 (6) |
| C25  | 0.762728 | -0.007587 | 0.084008 | 0.063*    |
| H25  | 0.72304 (13) | 0.06933 (12) | 0.12953 (8) | 0.0457 (5) |
| C26  | 0.712741 | 0.101362 | 0.100306 | 0.055*    |
| S2   | 0.03954 (3) | 0.33246 (3) | 0.57578 (2) | 0.04351 (13) |
| O3   | 0.32420 (9) | 0.25977 (11) | 0.43995 (7) | 0.0637 (5) |
| O4   | -0.09694 (9) | 0.43274 (9) | 0.46759 (6) | 0.0517 (4) |
| N4   | 0.16909 (9) | 0.27160 (10) | 0.57169 (6) | 0.0387 (4) |
| N5   | 0.01371 (10) | 0.37310 (11) | 0.41885 (6) | 0.0463 (4) |
| H5A  | -0.020564 | 0.407740 | 0.416974 | 0.056*    |
| H5B  | 0.047379 | 0.373820 | 0.394320 | 0.056*    |
| N6   | -0.09656 (9) | 0.42275 (9) | 0.55974 (6) | 0.0385 (4) |
| H6D  | -0.073302 | 0.401715 | 0.589899 | 0.046*    |
| C26  | 0.22238 (10) | 0.24755 (11) | 0.54371 (7) | 0.0369 (4) |
| C27  | 0.21831 (10) | 0.25553 (10) | 0.48685 (7) | 0.0331 (4) |
| C28  | 0.15804 (10) | 0.28521 (11) | 0.45707 (7) | 0.0346 (4) |
| C29  | 0.10163 (10) | 0.31114 (10) | 0.48631 (7) | 0.0298 (4) |
| C30  | 0.11108 (10) | 0.30046 (10) | 0.54284 (7) | 0.0331 (4) |
| C31  | 0.28697 (13) | 0.21482 (16) | 0.57694 (9) | 0.0592 (7) |
| H31A | 0.288331 | 0.230208 | 0.614884 | 0.089*    |
| H31B | 0.332503 | 0.228994 | 0.562430 | 0.089*    |
| H31C | 0.282312 | 0.163852 | 0.575239 | 0.089*    |
| C32  | 0.27920 (11) | 0.22264 (13) | 0.45800 (7) | 0.0431 (5) |
| C33  | 0.28079 (16) | 0.14500 (16) | 0.45355 (13) | 0.0716 (8) |
| C34  | 0.15891 (12) | 0.28910 (13) | 0.39694 (8) | 0.0449 (5) |
| H34  | 0.201552 | 0.308062 | 0.383690 | 0.054*    |
| Atom | U1  | U2  | U3  | U12  |
|------|-----|-----|-----|------|
| C35  | 0.10510 (12) | 0.26828 (12) | 0.36074 (8) | 0.0422 (5) |
| H35  | 0.059907 | 0.256078 | 0.373944 | 0.051* |
| C36  | 0.10852 (12) | 0.26214 (11) | 0.30152 (8) | 0.0396 (4) |
| C37  | 0.17197 (12) | 0.27616 (12) | 0.27676 (8) | 0.0449 (5) |
| H37  | 0.214360 | 0.294217 | 0.297862 | 0.054* |
| C38  | 0.17354 (12) | 0.26388 (14) | 0.22140 (8) | 0.0514 (6) |
| H38  | 0.216954 | 0.273184 | 0.204739 | 0.062* |
| C39  | 0.11155 (12) | 0.23804 (12) | 0.19073 (8) | 0.0425 (5) |
| H39  | 0.112564 | 0.228469 | 0.153073 | 0.051* |
| C40  | 0.04855 (12) | 0.22627 (11) | 0.21489 (8) | 0.0417 (5) |
| H40  | 0.005492 | 0.210072 | 0.193532 | 0.050* |
| C41  | 0.04721 (12) | 0.23769 (11) | 0.26968 (9) | 0.0423 (5) |
| H41  | 0.003374 | 0.228602 | 0.285860 | 0.051* |
| C42  | 0.03557 (10) | 0.35116 (10) | 0.47085 (7) | 0.0333 (4) |
| C43  | −0.00274 (10) | 0.36595 (10) | 0.51460 (7) | 0.0338 (4) |
| C44  | −0.06858 (11) | 0.40936 (11) | 0.51163 (8) | 0.0369 (4) |
| C45  | −0.15844 (11) | 0.46469 (11) | 0.56711 (8) | 0.0406 (4) |
| C46  | −0.19320 (13) | 0.45263 (16) | 0.61369 (9) | 0.0573 (6) |
| H46  | −0.176193 | 0.416450 | 0.638244 | 0.069* |
| C47  | −0.25276 (14) | 0.49358 (18) | 0.62416 (11) | 0.0707 (8) |
| H47  | −0.275922 | 0.485663 | 0.656211 | 0.085* |
| C48  | −0.27856 (14) | 0.54561 (16) | 0.58849 (12) | 0.0647 (7) |
| H48  | −0.319212 | 0.573612 | 0.595885 | 0.078* |
| C49  | −0.24488 (13) | 0.55661 (13) | 0.54207 (12) | 0.0570 (6) |
| H49  | −0.263306 | 0.591860 | 0.517132 | 0.068* |
| C50  | −0.18451 (12) | 0.51725 (11) | 0.53093 (10) | 0.0473 (5) |
| H50  | −0.161260 | 0.526015 | 0.499054 | 0.057* |
| S3   | 0.41314 (3) | 0.24335 (2) | 0.18027 (2) | 0.03262 (10) |
| O5   | 0.55494 (9) | −0.03140 (9) | 0.31956 (7) | 0.0561 (4) |
| O6   | 0.34405 (8) | 0.37124 (7) | 0.28995 (5) | 0.0366 (3) |
| N7   | 0.46504 (9) | 0.11366 (8) | 0.18421 (6) | 0.0331 (3) |
| N8   | 0.38422 (9) | 0.24697 (9) | 0.33573 (6) | 0.0358 (4) |
| H8D  | 0.363500 | 0.289773 | 0.338965 | 0.043* |
| H8E  | 0.390783 | 0.218293 | 0.360412 | 0.043* |
| N9   | 0.33751 (8) | 0.38233 (8) | 0.19765 (6) | 0.0318 (3) |
| H9A  | 0.344208 | 0.362128 | 0.165217 | 0.038* |
| C51  | 0.48351 (10) | 0.05531 (10) | 0.21191 (7) | 0.0337 (4) |
| C52  | 0.47698 (10) | 0.04870 (10) | 0.26806 (7) | 0.0322 (4) |
| C53  | 0.45350 (10) | 0.10456 (9) | 0.29802 (7) | 0.0300 (4) |
| C54  | 0.43342 (9) | 0.16649 (9) | 0.26909 (7) | 0.0270 (3) |
| C55  | 0.44097 (9) | 0.16667 (9) | 0.21287 (7) | 0.0285 (3) |
| C56  | 0.51391 (14) | −0.00244 (12) | 0.17965 (9) | 0.0495 (5) |
| H56A | 0.494565 | −0.047394 | 0.190622 | 0.074* |
| H56B | 0.567744 | −0.002688 | 0.186584 | 0.074* |
| H56C | 0.499232 | 0.005148 | 0.140725 | 0.074* |
| C57  | 0.49572 (11) | −0.02065 (10) | 0.29534 (8) | 0.0375 (4) |
| C58  | 0.43791 (16) | −0.07515 (13) | 0.28970 (14) | 0.0694 (8) |
| H58A | 0.402642 | −0.066499 | 0.316094 | 0.104* |
| Atom  | x      | y      | z      | Ueq   |
|-------|--------|--------|--------|-------|
| H58B  | 0.460575 | -0.121146 | 0.296565 | 0.104* |
| H58C  | 0.412261 | -0.073868 | 0.252722 | 0.104* |
| C59   | 0.44971 (11) | 0.09547 (10) | 0.35740 (7) | 0.0351 (4) |
| H59   | 0.420414 | 0.058376 | 0.368735 | 0.042* |
| C60   | 0.48473 (10) | 0.13597 (10) | 0.39578 (7) | 0.0348 (4) |
| H60   | 0.514138 | 0.172461 | 0.383629 | 0.042* |
| C61   | 0.48267 (10) | 0.13014 (11) | 0.45512 (7) | 0.0351 (4) |
| C62   | 0.51007 (11) | 0.18508 (13) | 0.48754 (8) | 0.0441 (5) |
| H62   | 0.532423 | 0.223576 | 0.471510 | 0.053* |
| C63   | 0.50531 (14) | 0.18468 (14) | 0.54312 (9) | 0.0538 (6) |
| H63   | 0.524141 | 0.229777 | 0.564808 | 0.065* |
| C64   | 0.47365 (14) | 0.12944 (14) | 0.56708 (8) | 0.0526 (6) |
| H64   | 0.469875 | 0.129730 | 0.605133 | 0.063* |
| C65   | 0.44757 (17) | 0.07403 (15) | 0.53596 (10) | 0.0637 (7) |
| H65   | 0.426479 | 0.035234 | 0.552525 | 0.076* |
| C66   | 0.45179 (16) | 0.07417 (13) | 0.47981 (9) | 0.0562 (6) |
| H66   | 0.433295 | 0.035497 | 0.458403 | 0.067* |
| C67   | 0.40131 (9) | 0.23191 (9) | 0.28491 (7) | 0.0275 (3) |
| C68   | 0.38802 (9) | 0.27729 (9) | 0.24124 (7) | 0.0285 (3) |
| C69   | 0.35528 (9) | 0.34646 (9) | 0.24508 (7) | 0.0295 (4) |
| C70   | 0.31164 (10) | 0.45239 (10) | 0.19555 (7) | 0.0326 (4) |
| C71   | 0.25865 (11) | 0.47501 (11) | 0.22759 (8) | 0.0394 (4) |
| H71   | 0.237517 | 0.443184 | 0.250946 | 0.047* |
| C72   | 0.23663 (12) | 0.54441 (12) | 0.22536 (9) | 0.0483 (5) |
| H72   | 0.200382 | 0.559884 | 0.247398 | 0.058* |
| C73   | 0.26680 (14) | 0.59137 (12) | 0.19145 (10) | 0.0528 (6) |
| H73   | 0.251683 | 0.638872 | 0.190318 | 0.063* |
| C74   | 0.31914 (14) | 0.56837 (12) | 0.15928 (10) | 0.0535 (6) |
| H74   | 0.340186 | 0.600310 | 0.135956 | 0.064* |
| C75   | 0.34120 (12) | 0.49912 (11) | 0.16073 (8) | 0.0421 (5) |
| H75   | 0.376527 | 0.483546 | 0.137950 | 0.051* |
| S4    | 0.96809 (2) | 0.10829 (3) | 0.58282 (2) | 0.03352 (11) |
| O7    | 0.66763 (8) | 0.24504 (8) | 0.44738 (6) | 0.0469 (4) |
| O8    | 1.10998 (8) | 0.08556 (9) | 0.47378 (6) | 0.0525 (4) |
| N10   | 0.83433 (8) | 0.16708 (9) | 0.57761 (6) | 0.0320 (3) |
| N11   | 0.99537 (9) | 0.16551 (9) | 0.43311 (6) | 0.0394 (4) |
| H11A  | 1.035436 | 0.139938 | 0.426578 | 0.047* |
| H11B  | 0.958515 | 0.174776 | 0.406215 | 0.047* |
| N12   | 1.11828 (8) | 0.04831 (9) | 0.56184 (7) | 0.0361 (3) |
| H12A  | 1.100106 | 0.051922 | 0.594580 | 0.043* |
| C76   | 0.77995 (10) | 0.20337 (11) | 0.55000 (7) | 0.0338 (4) |
| C77   | 0.78529 (10) | 0.22969 (10) | 0.49697 (7) | 0.0305 (4) |
| C78   | 0.84814 (9) | 0.21799 (9) | 0.47142 (7) | 0.0283 (3) |
| C79   | 0.90435 (9) | 0.17761 (9) | 0.49958 (7) | 0.0280 (3) |
| C80   | 0.89395 (9) | 0.15499 (9) | 0.55204 (7) | 0.0289 (3) |
| C81   | 0.71284 (12) | 0.21607 (14) | 0.57828 (8) | 0.0506 (6) |
| H81A  | 0.714743 | 0.186665 | 0.610886 | 0.076* |
| H81B  | 0.668763 | 0.204530 | 0.553632 | 0.076* |
|           | U^{11}       | U^{22}       | U^{33}       | U^{12}      | U^{13}      | U^{23}       |
|-----------|--------------|--------------|--------------|-------------|-------------|--------------|
| S1        | 0.0399 (2)   | 0.0355 (2)   | 0.02096 (19) | 0.00223 (18)| 0.00724 (17)| 0.00067 (17)|
| O1        | 0.0468 (8)   | 0.0355 (7)   | 0.0432 (8)   | 0.0021 (6)  | 0.0021 (6)  | 0.00060 (6)  |
| O2        | 0.0534 (8)   | 0.0395 (7)   | 0.0312 (7)   | 0.0106 (6)  | 0.0155 (6)  | 0.0081 (6)   |
| N1        | 0.0308 (7)   | 0.0337 (8)   | 0.0252 (7)   | 0.0029 (6)  | 0.0023 (6)  | 0.0020 (6)   |
| N2        | 0.0406 (8)   | 0.0357 (8)   | 0.0217 (7)   | 0.0038 (6)  | 0.0074 (6)  | 0.0029 (6)   |
| N3        | 0.0376 (8)   | 0.0352 (8)   | 0.0234 (7)   | 0.0021 (6)  | 0.0046 (6)  | 0.0009 (6)   |
| C1        | 0.0312 (8)   | 0.0328 (9)   | 0.0280 (9)   | 0.0028 (7)  | 0.0016 (7)  | 0.0000 (7)   |
| C2        | 0.0303 (8)   | 0.0323 (9)   | 0.0271 (8)   | 0.0012 (7)  | 0.0022 (7)  | 0.0018 (7)   |
| C3        | 0.0273 (8)   | 0.0331 (9)   | 0.0237 (8)   | 0.0025 (7)  | 0.0015 (6)  | 0.0016 (7)   |

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|  | x       | y       | z       | U11     | U22     | U33     | U12     | U13     | U23     |
|---|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| C4 | 0.0253  | 0.0319  | 0.0219  | -0.0028 | 0.0019  | -0.0002 |
| C5 | 0.0286  | 0.0336  | 0.0212  | -0.0032 | 0.0022  | -0.0002 |
| C6 | 0.0510  | 0.0356  | 0.0385  | 0.0007  | 0.0067  | 0.0068  |
| C7 | 0.0407  | 0.0325  | 0.0258  | 0.0034  | 0.0034  | 0.0020  |
| C8 | 0.0413  | 0.0442  | 0.0393  | 0.0052  | 0.0072  | -0.0041 |
| C9 | 0.0317  | 0.0331  | 0.0271  | 0.0010  | 0.0063  | -0.0005 |
| C10| 0.0326  | 0.0346  | 0.0274  | 0.0023  | 0.0047  | -0.0010 |
| C11| 0.0381  | 0.0340  | 0.0260  | 0.0078  | 0.0073  | -0.0037 |
| C12| 0.0438  | 0.0431  | 0.0294  | 0.0019  | 0.0029  | -0.0063 |
| C13| 0.0639  | 0.0508  | 0.0280  | 0.0042  | 0.0044  | -0.0082 |
| C14| 0.0785  | 0.0492  | 0.0273  | 0.0048  | 0.0155  | -0.0026 |
| C15| 0.0649  | 0.0475  | 0.0383  | -0.0066 | 0.0225  | -0.0030 |
| C16| 0.0481  | 0.0415  | 0.0290  | -0.0015 | 0.0101  | -0.0060 |
| C17| 0.0253  | 0.0337  | 0.0219  | -0.0019 | 0.0035  | 0.0011  |
| C18| 0.0297  | 0.0352  | 0.0230  | 0.0002  | 0.0038  | 0.0005  |
| C19| 0.0290  | 0.0376  | 0.0260  | 0.0006  | 0.0049  | -0.0014 |
| C20| 0.0285  | 0.0354  | 0.0306  | -0.0012 | 0.0040  | -0.0051 |
| C21| 0.0466  | 0.0403  | 0.0328  | 0.0062  | 0.0043  | -0.0021 |
| C22| 0.0450  | 0.0412  | 0.0407  | 0.0068  | 0.0014  | -0.0020 |
| C23| 0.0408  | 0.0424  | 0.0486  | 0.0077  | 0.0008  | -0.0101 |
| C24| 0.0654  | 0.0561  | 0.0375  | 0.0179  | 0.0094  | -0.0092 |
| C25| 0.0564  | 0.0488  | 0.0326  | 0.0129  | 0.0080  | -0.0023 |
| S2 | 0.0389  | 0.0704  | 0.0227  | 0.0162  | 0.00994 | 0.0093  |
| O3 | 0.0500  | 0.0958  | 0.0501  | 0.0059  | 0.0272  | 0.0143  |
| O4 | 0.0491  | 0.0733  | 0.0321  | 0.0219  | 0.0018  | 0.0049  |
| N4 | 0.0362  | 0.0592  | 0.0210  | 0.0114  | 0.0053  | 0.0049  |
| N5 | 0.0486  | 0.0675  | 0.0227  | 0.0173  | 0.0042  | 0.0064  |
| N6 | 0.0338  | 0.0524  | 0.0292  | 0.0076  | 0.0037  | 0.0003  |
| C26| 0.0341  | 0.0543  | 0.0226  | 0.0038  | 0.0048  | 0.0006  |
| C27| 0.0306  | 0.0475  | 0.0218  | -0.0023 | 0.0052  | -0.0029 |
| C28| 0.0353  | 0.0476  | 0.0214  | -0.0012 | 0.0053  | -0.0007 |
| C29| 0.0309  | 0.0378  | 0.0204  | -0.0043 | 0.0017  | 0.0012  |
| C30| 0.0343  | 0.0443  | 0.0213  | -0.0001 | 0.0061  | 0.0045  |
| C31| 0.0503  | 0.0982  | 0.0289  | 0.0291  | 0.0016  | -0.0006 |
| C32| 0.0328  | 0.0751  | 0.0214  | 0.0036  | 0.0027  | -0.0046 |
| C33| 0.0606  | 0.0814  | 0.0758  | 0.0055  | 0.0199  | -0.0332 |
| C34| 0.0426  | 0.0654  | 0.0269  | 0.0016  | 0.0056  | 0.0013  |
| C35| 0.0399  | 0.0528  | 0.0351  | -0.0063 | 0.0087  | 0.0004  |
| C36| 0.0518  | 0.0409  | 0.0271  | 0.0030  | 0.0084  | 0.0017  |
| C37| 0.0471  | 0.0560  | 0.0292  | -0.0133 | 0.0063  | -0.0006 |
| C38| 0.0434  | 0.0829  | 0.0284  | -0.0175 | 0.0064  | 0.0038  |
| C39| 0.0470  | 0.0585  | 0.0229  | -0.0094 | 0.0072  | -0.0087 |
| C40| 0.0455  | 0.0439  | 0.0360  | -0.0078 | 0.0055  | -0.0056 |
| C41| 0.0439  | 0.0450  | 0.0394  | -0.0031 | 0.0111  | 0.0007  |
| C42| 0.0352  | 0.0413  | 0.0229  | -0.0020 | 0.0014  | 0.0022  |
| C43| 0.0335  | 0.0441  | 0.0239  | 0.0007  | 0.0035  | 0.0033  |
| C44| 0.0355  | 0.0466  | 0.0284  | 0.0022  | 0.0025  | 0.0009  |
| C45| 0.0335  | 0.0486  | 0.0392  | 0.0012  | 0.0010  | -0.0112 |
| Atom | U1  | U2  | U3  | U4  | U5  | U6  |
|------|-----|-----|-----|-----|-----|-----|
| C46  | 0.0418 (11) | 0.0942 (19) | 0.0361 (11) | 0.0164 (12) | 0.0057 (9) | −0.0009 (12) |
| C47  | 0.0483 (13) | 0.114 (2) | 0.0505 (14) | 0.0213 (15) | 0.0103 (11) | −0.0146 (15) |
| C48  | 0.0429 (12) | 0.0757 (18) | 0.0747 (18) | 0.0148 (12) | 0.0025 (12) | −0.0252 (15) |
| C49  | 0.0482 (13) | 0.0444 (12) | 0.0765 (17) | 0.0051 (10) | −0.0014 (12) | −0.0089 (12) |
| C50  | 0.0426 (11) | 0.0405 (11) | 0.0587 (14) | 0.0005 (9) | 0.0050 (10) | −0.0040 (10) |
| S3   | 0.0428 (2) | 0.0355 (2) | 0.0206 (2) | 0.00549 (18) | 0.00827 (17) | 0.0122 (17) |
| O5   | 0.0571 (10) | 0.0566 (10) | 0.0516 (9) | 0.0090 (8) | −0.0073 (8) | 0.0142 (8) |
| O6   | 0.0463 (7) | 0.0397 (7) | 0.0243 (6) | 0.0089 (6) | 0.0062 (5) | −0.0027 (5) |
| N7   | 0.0393 (8) | 0.0370 (8) | 0.0232 (7) | 0.0047 (7) | 0.0047 (6) | −0.0041 (6) |
| N8   | 0.0488 (9) | 0.0388 (8) | 0.0212 (7) | 0.0105 (7) | 0.0103 (6) | 0.0022 (6) |
| N9   | 0.0373 (8) | 0.0353 (8) | 0.0232 (7) | 0.0046 (6) | 0.0054 (6) | −0.0004 (6) |
| C51  | 0.0339 (9) | 0.0340 (9) | 0.0283 (9) | 0.0007 (7) | 0.0011 (7) | −0.0012 (7) |
| C52  | 0.0310 (8) | 0.0338 (9) | 0.0251 (8) | −0.0005 (7) | 0.0034 (7) | −0.0013 (7) |
| C54  | 0.0377 (9) | 0.0351 (9) | 0.0279 (9) | 0.0033 (8) | 0.0026 (7) | −0.0048 (7) |
| C55  | 0.0333 (9) | 0.0340 (9) | 0.0283 (9) | 0.0007 (7) | 0.0011 (7) | −0.0012 (7) |
| C56  | 0.0339 (9) | 0.0340 (9) | 0.0283 (9) | 0.0007 (7) | 0.0011 (7) | −0.0012 (7) |
| C57  | 0.0310 (8) | 0.0338 (9) | 0.0251 (8) | −0.0005 (7) | 0.0034 (7) | −0.0013 (7) |
| C58  | 0.0377 (9) | 0.0351 (9) | 0.0279 (9) | 0.0033 (8) | 0.0026 (7) | −0.0048 (7) |
| C59  | 0.0333 (9) | 0.0340 (9) | 0.0283 (9) | 0.0007 (7) | 0.0011 (7) | −0.0012 (7) |
| C60  | 0.0339 (9) | 0.0340 (9) | 0.0283 (9) | 0.0007 (7) | 0.0011 (7) | −0.0012 (7) |
| C61  | 0.0310 (8) | 0.0338 (9) | 0.0251 (8) | −0.0005 (7) | 0.0034 (7) | −0.0013 (7) |
| C62  | 0.0377 (9) | 0.0351 (9) | 0.0279 (9) | 0.0033 (8) | 0.0026 (7) | −0.0048 (7) |
| C63  | 0.0333 (9) | 0.0340 (9) | 0.0283 (9) | 0.0007 (7) | 0.0011 (7) | −0.0012 (7) |
| C64  | 0.0339 (9) | 0.0340 (9) | 0.0283 (9) | 0.0007 (7) | 0.0011 (7) | −0.0012 (7) |
| C65  | 0.0310 (8) | 0.0338 (9) | 0.0251 (8) | −0.0005 (7) | 0.0034 (7) | −0.0013 (7) |
| C66  | 0.0377 (9) | 0.0351 (9) | 0.0279 (9) | 0.0033 (8) | 0.0026 (7) | −0.0048 (7) |
| C67  | 0.0333 (9) | 0.0340 (9) | 0.0283 (9) | 0.0007 (7) | 0.0011 (7) | −0.0012 (7) |
| C68  | 0.0310 (8) | 0.0338 (9) | 0.0251 (8) | −0.0005 (7) | 0.0034 (7) | −0.0013 (7) |
| C69  | 0.0377 (9) | 0.0351 (9) | 0.0279 (9) | 0.0033 (8) | 0.0026 (7) | −0.0048 (7) |
| C70  | 0.0333 (9) | 0.0340 (9) | 0.0283 (9) | 0.0007 (7) | 0.0011 (7) | −0.0012 (7) |
| C71  | 0.0310 (8) | 0.0338 (9) | 0.0251 (8) | −0.0005 (7) | 0.0034 (7) | −0.0013 (7) |
| C72  | 0.0377 (9) | 0.0351 (9) | 0.0279 (9) | 0.0033 (8) | 0.0026 (7) | −0.0048 (7) |
### Geometric parameters (Å, °)

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| C82 | 0.0312 (9) | 0.0463 (11) | 0.0257 (9) | 0.0056 (8) | 0.0078 (7) | 0.0023 (8) |
| C83 | 0.0448 (11) | 0.0453 (12) | 0.0649 (15) | 0.0094 (10) | 0.0015 (11) | 0.0081 (11) |
| C84 | 0.0319 (9) | 0.0377 (9) | 0.0258 (9) | −0.0001 (7) | 0.0048 (7) | 0.0062 (7) |
| C85 | 0.0316 (9) | 0.0386 (10) | 0.0272 (9) | 0.0016 (7) | 0.0057 (7) | 0.0054 (7) |
| C86 | 0.0258 (8) | 0.0427 (10) | 0.0242 (8) | 0.0019 (7) | 0.0012 (6) | 0.0043 (7) |
| C87 | 0.0340 (9) | 0.0468 (11) | 0.0284 (9) | −0.0029 (8) | −0.0005 (7) | 0.0000 (8) |
| C88 | 0.0405 (10) | 0.0652 (14) | 0.0246 (9) | −0.0039 (10) | −0.0011 (8) | −0.0046 (9) |
| C89 | 0.0394 (10) | 0.0723 (15) | 0.0234 (9) | −0.0108 (10) | 0.0003 (8) | 0.0090 (9) |
| C90 | 0.0438 (11) | 0.0530 (12) | 0.0321 (10) | −0.0087 (9) | −0.0006 (8) | 0.0107 (9) |
| C91 | 0.0428 (10) | 0.0439 (11) | 0.0272 (9) | −0.0020 (8) | 0.0019 (8) | 0.0029 (8) |
| C92 | 0.0300 (8) | 0.0356 (9) | 0.0244 (8) | −0.0009 (7) | 0.0069 (7) | 0.0009 (7) |
| C93 | 0.0317 (9) | 0.0397 (10) | 0.0257 (8) | 0.0019 (7) | 0.0047 (7) | 0.0020 (7) |
| C94 | 0.0315 (9) | 0.0443 (10) | 0.0317 (9) | 0.0050 (8) | 0.0069 (7) | 0.0038 (8) |
| C95 | 0.0281 (8) | 0.0350 (9) | 0.0426 (10) | 0.0014 (7) | 0.0047 (8) | 0.0042 (8) |
| C96 | 0.0380 (10) | 0.0656 (14) | 0.0412 (11) | 0.0116 (10) | 0.0088 (9) | 0.0110 (10) |
| C97 | 0.0381 (11) | 0.0764 (17) | 0.0576 (14) | 0.0141 (11) | 0.0067 (10) | 0.0240 (13) |
| C98 | 0.0378 (11) | 0.0516 (13) | 0.0795 (17) | 0.0144 (10) | 0.0162 (11) | 0.0150 (12) |
| C99 | 0.0470 (12) | 0.0421 (12) | 0.0714 (16) | 0.0090 (10) | 0.0162 (11) | −0.0098 (11) |
| C100 | 0.0397 (10) | 0.0430 (11) | 0.0501 (12) | 0.0045 (9) | 0.0019 (9) | −0.0110 (9) |

**S1—C5**  1.7209 (18)  **S3—C55**  1.7241 (18)
**S1—C18**  1.7516 (18)  **S3—C68**  1.7471 (17)
**O1—C7**  1.212 (2)  **O5—C57**  1.195 (3)
**O2—C19**  1.238 (2)  **O6—C69**  1.243 (2)
**N1—C1**  1.339 (2)  **N7—C51**  1.334 (2)
**N1—C5**  1.340 (2)  **N7—C55**  1.339 (2)
**N2—C17**  1.375 (2)  **N8—C67**  1.357 (2)
**N2—H2A**  0.9100  **N8—H8D**  0.9100
**N2—H2B**  0.9099  **N8—H8E**  0.8193
**N3—C19**  1.368 (2)  **N9—C69**  1.366 (2)
**N3—C20**  1.415 (2)  **N9—C70**  1.421 (2)
**N3—H3A**  0.9100  **N9—H9A**  0.9100
**C1—C2**  1.414 (2)  **C51—C52**  1.411 (3)
**C1—C6**  1.504 (3)  **C51—C56**  1.505 (3)
**C2—C3**  1.397 (2)  **C52—C53**  1.395 (3)
**C2—C7**  1.509 (2)  **C52—C57**  1.511 (3)
**C3—C4**  1.410 (2)  **C53—C54**  1.412 (2)
**C3—C9**  1.476 (2)  **C53—C59**  1.486 (2)
**C4—C5**  1.405 (2)  **C54—C55**  1.410 (2)
**C4—C17**  1.447 (2)  **C54—C67**  1.455 (2)
**C6—H6A**  0.9800  **C56—H56A**  0.9800
**C6—H6B**  0.9800  **C56—H56B**  0.9800
**C6—H6C**  0.9800  **C56—H56C**  0.9800
**C7—C8**  1.491 (3)  **C57—C58**  1.480 (3)
**C8—H8A**  0.9800  **C58—H58A**  0.9800
**C8—H8B**  0.9800  **C58—H58B**  0.9800
| Bond          | Distance       | Bond          | Distance       |
|--------------|----------------|--------------|----------------|
| C8—H8C       | 0.9800         | C58—H58C     | 0.9800         |
| C9—C10       | 1.337 (3)      | C59—C60      | 1.333 (3)      |
| C9—H9        | 0.9500         | C59—H59      | 0.9500         |
| C10—C11      | 1.467 (2)      | C60—C61      | 1.474 (2)      |
| C10—H10      | 0.9500         | C60—H60      | 0.9500         |
| C11—C16      | 1.390 (3)      | C61—C62      | 1.382 (3)      |
| C11—C12      | 1.398 (3)      | C61—C66      | 1.384 (3)      |
| C12—C13      | 1.383 (3)      | C62—C63      | 1.385 (3)      |
| C12—H12      | 0.9500         | C62—H62      | 0.9500         |
| C13—C14      | 1.373 (3)      | C63—C64      | 1.371 (4)      |
| C13—H13      | 0.9500         | C63—H63      | 0.9500         |
| C14—C15      | 1.387 (3)      | C64—C65      | 1.365 (4)      |
| C14—H14      | 0.9500         | C64—H64      | 0.9500         |
| C15—C16      | 1.388 (3)      | C65—C66      | 1.397 (3)      |
| C15—H15      | 0.9500         | C65—H65      | 0.9500         |
| C16—H16      | 0.9500         | C66—H66      | 0.9500         |
| C17—C18      | 1.385 (2)      | C67—C68      | 1.385 (2)      |
| C18—C19      | 1.460 (3)      | C68—C69      | 1.461 (2)      |
| C20—C25      | 1.387 (3)      | C70—C71      | 1.386 (3)      |
| C20—C21      | 1.394 (3)      | C70—C75      | 1.391 (3)      |
| C21—C22      | 1.388 (3)      | C71—C72      | 1.388 (3)      |
| C21—H21      | 0.9500         | C71—H71      | 0.9500         |
| C22—C23      | 1.378 (3)      | C72—C73      | 1.384 (3)      |
| C22—H22      | 0.9500         | C72—H72      | 0.9500         |
| C23—C24      | 1.371 (3)      | C73—C74      | 1.381 (3)      |
| C23—H23      | 0.9500         | C73—H73      | 0.9500         |
| C24—C25      | 1.389 (3)      | C74—C75      | 1.385 (3)      |
| C24—H24      | 0.9500         | C74—H74      | 0.9500         |
| C25—H25      | 0.9500         | C75—H75      | 0.9500         |
| S2—C30       | 1.7267 (19)    | S4—C80       | 1.7282 (18)    |
| S2—C43       | 1.7420 (18)    | S4—C93       | 1.7548 (18)    |
| O3—C32       | 1.209 (3)      | O7—C82       | 1.208 (2)      |
| O4—C44       | 1.236 (2)      | O8—C94       | 1.237 (2)      |
| N4—C30       | 1.331 (2)      | N10—C76      | 1.337 (2)      |
| N4—C26       | 1.337 (2)      | N10—C80      | 1.339 (2)      |
| N5—C42       | 1.368 (2)      | N11—C92      | 1.368 (2)      |
| N5—H5A       | 0.9100         | N11—H11A     | 0.9100         |
| N5—H5B       | 0.9100         | N11—H11B     | 0.9099         |
| N6—C44       | 1.369 (2)      | N12—C94      | 1.360 (2)      |
| N6—C45       | 1.415 (3)      | N12—C95      | 1.422 (2)      |
| N6—H6D       | 0.9099         | N12—H12A     | 0.9099         |
| C26—C27      | 1.403 (2)      | C76—C77      | 1.417 (2)      |
| C26—C31      | 1.499 (3)      | C76—C81      | 1.497 (3)      |
| C27—C28      | 1.394 (3)      | C77—C78      | 1.388 (2)      |
| C27—C32      | 1.507 (3)      | C77—C82      | 1.511 (2)      |
| C28—C29      | 1.412 (3)      | C78—C79      | 1.407 (2)      |
| C28—C34      | 1.489 (3)      | C78—C84      | 1.485 (2)      |
| C29—C30      | 1.403 (2)      | C79—C80      | 1.399 (2)      |
C29—C42 1.445 (3)  C79—C92 1.444 (2)
C31—H31A 0.9800  C81—H81A 0.9800
C31—H31B 0.9800  C81—H81B 0.9800
C31—H31C 0.9800  C81—H81C 0.9800
C32—C33 1.491 (4)  C82—C83 1.489 (3)
C33—H33A 0.9800  C83—H83A 0.9800
C33—H33B 0.9800  C83—H83B 0.9800
C33—H33C 0.9800  C83—H83C 0.9800
C34—C35 1.316 (3)  C84—C85 1.333 (3)
C34—H34 0.9500  C84—H84 0.9500
C35—C36 1.475 (3)  C85—C86 1.475 (2)
C35—H35 0.9500  C85—H85 0.9500
C36—C41 1.378 (3)  C86—C87 1.392 (3)
C36—C37 1.395 (3)  C86—C91 1.393 (3)
C37—C38 1.391 (3)  C87—C88 1.387 (3)
C37—H37 0.9500  C87—H87 0.9500
C38—C39 1.383 (3)  C88—C89 1.381 (3)
C38—H38 0.9500  C88—H88 0.9500
C39—C40 1.373 (3)  C89—C90 1.380 (3)
C39—H39 0.9500  C89—H90 0.9500
C40—C41 1.374 (3)  C90—C91 1.386 (3)
C40—H40 0.9500  C90—H90 0.9500
C41—H41 0.9500  C91—H91 0.9500
C42—C43 1.380 (3)  C92—C93 1.372 (3)
C43—C44 1.458 (3)  C93—C94 1.464 (3)
C45—C46 1.393 (3)  C95—C96 1.385 (3)
C45—C50 1.394 (3)  C95—C100 1.389 (3)
C46—C47 1.389 (3)  C96—C97 1.388 (3)
C46—H46 0.9500  C96—H96 0.9500
C47—C48 1.378 (4)  C97—C98 1.374 (4)
C47—H47 0.9500  C97—H97 0.9500
C48—C49 1.376 (4)  C98—C99 1.371 (4)
C48—H48 0.9500  C98—H98 0.9500
C49—C50 1.389 (3)  C99—C100 1.392 (3)
C49—H49 0.9500  C99—H99 0.9500
C50—H50 0.9500  C100—H100 0.9500

C5—S1—C18 90.75 (8)  C55—S3—C68 90.36 (8)
C1—N1—C5 116.36 (15)  C51—N7—C55 116.29 (16)
C17—N2—H2A 111.9  C67—N8—H8D 114.4
C17—N2—H2B 114.7  C67—N8—H8E 121.1
H2A—N2—H2B 118.6  H8D—N8—H8E 124.5
C19—N3—C20 127.14 (16)  C69—N9—C70 123.54 (15)
C19—N3—H3A 116.7  C69—N9—H9A 119.9
C20—N3—H3A 116.1  C70—N9—H9A 116.5
N1—C1—C2 122.45 (16)  N7—C51—C52 122.36 (16)
N1—C1—C6 115.68 (16)  N7—C51—C56 115.55 (16)
C2—C1—C6 121.85 (17)  C52—C51—C56 122.07 (17)
C3—C2—C1 120.65 (16)  C53—C52—C51 121.14 (17)
C3—C2—C7 121.03 (16)  C53—C52—C57 120.33 (16)
C1—C2—C7 118.32 (16)  C51—C52—C57 118.53 (16)
C2—C3—C4 117.10 (15)  C52—C53—C54 116.96 (16)
C2—C3—C9 122.21 (16)  C52—C53—C59 118.97 (16)
C4—C3—C9 120.69 (16)  C54—C53—C59 124.06 (16)
C5—C4—C3 117.37 (16)  C55—C54—C53 116.87 (16)
C5—C4—C17 111.20 (15)  C55—C54—C67 110.39 (15)
C3—C4—C17 131.42 (15)  C53—C54—C67 132.63 (15)
N1—C5—C4 125.97 (16)  N7—C55—C54 126.31 (16)
N1—C5—S1 120.74 (13)  N7—C55—S3 119.71 (13)
C4—C5—S1 113.96 (13)  C54—C55—S3 113.95 (13)
C1—C6—H6A 109.5  C51—C56—H56A 109.5
C1—C6—H6B 109.5  C51—C56—H56B 109.5
H6A—C6—H6B 109.5  H56A—C56—H56B 109.5
H6A—C6—H6C 109.5  H56A—C56—H56C 109.5
H6B—C6—H6C 109.5  H56B—C56—H56C 109.5
O1—C7—C8 123.00 (18)  O5—C57—C58 121.6 (2)
O1—C7—C2 119.96 (17)  O5—C57—C52 121.51 (19)
C8—C7—C2 116.97 (16)  C58—C57—C52 116.92 (18)
C7—C8—H8A 109.5  C57—C58—H58A 109.5
C7—C8—H8B 109.5  C57—C58—H58B 109.5
H8A—C8—H8B 109.5  H58A—C58—H58B 109.5
C7—C8—H8C 109.5  C57—C58—H58C 109.5
H8A—C8—H8C 109.5  H58A—C58—H58C 109.5
H8B—C8—H8C 109.5  H58B—C58—H58C 109.5
C10—C9—C3 125.12 (17)  C60—C59—C53 124.26 (18)
C10—C9—H9 117.4  C60—C59—H59 117.9
C3—C9—H9 117.4  C53—C59—H59 117.9
C9—C10—C11 125.34 (18)  C59—C60—C61 126.87 (18)
C9—C10—H10 117.3  C59—C60—H60 116.6
C11—C10—H10 117.3  C61—C60—H60 116.6
C16—C11—C12 118.37 (17)  C62—C61—C66 118.26 (18)
C16—C11—C10 122.68 (17)  C62—C61—C60 118.09 (18)
C12—C11—C10 118.96 (18)  C66—C61—C60 123.58 (19)
C13—C12—C11 120.8 (2)  C61—C62—C63 120.8 (2)
C13—C12—H12 119.6  C61—C62—H62 119.6
C11—C12—H12 119.6  C63—C62—H62 119.6
C14—C13—C12 120.1 (2)  C64—C63—C62 120.5 (2)
C14—C13—H13 119.9  C64—C63—H63 119.7
C12—C13—H13 119.9  C62—C63—H63 119.7
C13—C14—C15 120.1 (2)  C65—C64—C63 119.6 (2)
C13—C14—H14 119.9  C65—C64—H64 120.2
C15—C14—H14 119.9  C63—C64—H64 120.2
C14—C15—C16 119.8 (2)  C64—C65—C66 120.2 (2)
C14—C15—H15 120.1  C64—C65—H65 119.9
C16—C15—H15 120.1  C66—C65—H65 119.9

Acta Cryst. (2022). E78, 225-230
| Bond | Angle (deg) | Bond | Angle (deg) | Bond | Angle (deg) |
|------|------------|------|------------|------|------------|
| C15—C16—C11 | 120.75 (19) | C61—C66—C65 | 120.6 (2) |
| C15—C16—H16 | 119.6 | C61—C66—H66 | 119.7 |
| C11—C16—H16 | 119.6 | C65—C66—H66 | 119.7 |
| N2—C17—C18 | 124.20 (16) | N8—C67—C68 | 123.25 (16) |
| N2—C17—C4 | 123.94 (15) | N8—C67—C54 | 124.88 (16) |
| C18—C17—C4 | 111.85 (15) | C68—C67—C54 | 111.85 (15) |
| C17—C18—C19 | 123.53 (16) | C67—C68—C69 | 123.77 (15) |
| C17—C18—S1 | 112.81 (13) | C67—C68—S3 | 113.42 (13) |
| C19—C18—S1 | 123.56 (13) | C69—C68—S3 | 122.80 (13) |
| O2—C19—N3 | 122.30 (17) | O6—C69—N9 | 121.72 (16) |
| O2—C19—C18 | 120.57 (16) | O6—C69—C68 | 120.86 (16) |
| N3—C19—C18 | 117.13 (16) | N9—C69—C68 | 117.42 (15) |
| C25—C20—C21 | 118.67 (18) | C71—C70—C75 | 119.70 (18) |
| C25—C20—N3 | 117.25 (17) | C71—C70—N9 | 121.65 (17) |
| C21—C20—N3 | 124.06 (16) | C75—C70—N9 | 118.64 (17) |
| C22—C21—H21 | 119.81 (19) | C70—C71—C72 | 119.6 (2) |
| C22—C21—H21 | 120.1 | C70—C71—H71 | 120.2 |
| C20—C21—H21 | 120.1 | C72—C71—H71 | 120.2 |
| C23—C22—C21 | 121.1 (2) | C73—C72—C71 | 120.9 (2) |
| C23—C22—H22 | 119.4 | C73—C72—H72 | 119.6 |
| C21—C22—H22 | 119.4 | C71—C72—H72 | 119.6 |
| C24—C23—C22 | 119.2 (2) | C74—C73—C72 | 119.2 (2) |
| C24—C23—H23 | 120.4 | C74—C73—H73 | 120.4 |
| C22—C23—H23 | 120.4 | C72—C73—H73 | 120.4 |
| C23—C24—C25 | 120.6 (2) | C73—C74—C75 | 120.6 (2) |
| C23—C24—H24 | 119.7 | C73—C74—H74 | 119.7 |
| C25—C24—H24 | 119.7 | C75—C74—H74 | 119.7 |
| C20—C25—C24 | 120.6 (2) | C74—C75—C70 | 120.0 (2) |
| C20—C25—H25 | 119.7 | C74—C75—H75 | 120.0 |
| C24—C25—H25 | 119.7 | C70—C75—H75 | 120.0 |
| C30—S2—C43 | 90.49 (9) | C80—S4—C93 | 90.64 (8) |
| C30—N4—C26 | 116.71 (15) | C76—N10—C80 | 116.58 (15) |
| C42—N5—H5A | 113.6 | C92—N11—H11A | 112.9 |
| C42—N5—H5B | 118.7 | C92—N11—H11B | 115.3 |
| H5A—N5—H5B | 117.9 | H11A—N11—H11B | 121.4 |
| C44—N6—C45 | 126.74 (17) | C94—N12—C95 | 125.78 (16) |
| C44—N6—H6D | 116.3 | C94—N12—H12A | 119.5 |
| C45—N6—H6D | 117.0 | C95—N12—H12A | 114.6 |
| N4—C26—C27 | 121.87 (17) | N10—C76—C77 | 122.25 (16) |
| N4—C26—C31 | 115.84 (16) | N10—C76—C81 | 116.61 (16) |
| C27—C26—C31 | 122.28 (17) | C77—C76—C81 | 121.14 (17) |
| C28—C27—C26 | 121.02 (17) | C78—C77—C76 | 120.50 (16) |
| C28—C27—C32 | 120.20 (16) | C78—C77—C82 | 119.46 (15) |
| C26—C27—C32 | 118.74 (17) | C76—C77—C82 | 120.02 (15) |
| C27—C28—C29 | 117.52 (16) | C77—C78—C79 | 117.36 (15) |
| C27—C28—C34 | 116.96 (17) | C77—C78—C84 | 121.77 (16) |
| C29—C28—C34 | 125.52 (17) | C79—C78—C84 | 120.87 (15) |
| C30—C29—C28 | 116.16 (16) | C80—C79—C78 | 117.50 (15) |
C30—C29—C42 110.35 (16) C80—C79—C92 111.56 (15)
C28—C29—C42 133.38 (16) C78—C79—C92 130.93 (16)
N4—C30—C29 126.64 (17) N10—C80—C79 125.75 (16)
N4—C30—S2 119.69 (13) N10—C80—S4 121.44 (13)
C29—C30—S2 113.61 (14) C79—C80—S4 112.81 (16)
C26—C31—H31A 109.5 C76—C81—H81A 109.5
C26—C31—H31B 109.5 C76—C81—H81B 109.5
H31A—C31—H31B 109.5 C76—C81—H81C 109.5
H31A—C31—H31C 109.5 H81A—C81—H81C 109.5
H31B—C31—H31C 109.5 H81B—C81—H81C 109.5
O3—C32—C33 122.7 (2) O7—C82—C83 122.19 (18)
O3—C32—C27 120.8 (2) O7—C82—C77 121.10 (18)
C33—C32—C27 116.6 (2) C83—C82—C77 116.70 (17)
C32—C33—H33A 109.5 C82—C83—C78 124.27 (17)
C32—C33—H33B 109.5 C82—C83—C84 117.9
H33A—C33—H33B 109.5 C82—C83—H83A 117.9
C32—C33—H33C 109.5 C82—C83—H83B 117.9
H33A—C33—H33C 109.5 C82—C83—H83C 117.9
H33B—C33—H33C 109.5 C83—C84—C85 122.96 (17)
C35—C34—C28 125.0 (2) C85—C84—C86 118.5
C35—C34—H34 117.5 C85—C84—H84 118.5
C28—C34—H34 117.5 C84—C85—H85 118.5
C34—C35—C36 126.0 (2) C84—C85—C86 118.5
C34—C35—H35 117.0 C84—C85—H85 118.5
C36—C35—H35 117.0 C85—C86—H85 118.5
C41—C36—C37 118.56 (18) C37—C36—C35 118.59 (17)
C41—C36—C35 118.17 (19) C37—C36—C35 118.59 (17)
C36—C35—C37 123.17 (19) C37—C36—C35 123.17 (19)
C36—C35—H35 120.43 (19) C37—C36—C35 120.43 (19)
C38—C37—C36 119.8 C38—C37—H37 119.6
C38—C37—H37 119.8 C38—C37—H37 119.8
C39—C38—C37 119.6 (2) C39—C38—H38 119.6
C39—C38—H38 120.2 C39—C38—H38 120.2
C38—C39—C38 120.2 C38—C39—H38 120.2
C40—C39—C38 119.76 (18) C40—C39—H39 119.87 (18)
C40—C39—H39 120.1 C40—C39—H39 120.1
C38—C39—H39 120.1 C38—C39—H39 120.1
C39—C40—C41 120.6 (2) C39—C40—C41 120.6 (2)
C39—C40—H40 119.7 C39—C40—H40 119.7
C40—C40—H40 119.7 C40—C40—H40 119.7
C40—C41—C36 120.97 (19) C40—C41—C36 120.97 (19)
C40—C41—H41 119.5 C40—C41—H41 119.5
C36—C41—H41 119.5 C36—C41—H41 119.5
N5—C42—C43 123.42 (18) N5—C42—C43 123.42 (18)
N5—C42—C29 124.04 (17) N5—C42—C29 124.04 (17)
C43—C42—C29 112.53 (16) C43—C42—C29 112.53 (16)
C42—C43—C44 124.40 (17) C42—C43—C44 124.40 (17)
C42—C43—S2: 112.87 (14)  C92—C93—S4: 112.75 (13)  
C44—C43—S2: 122.58 (14)  C94—C93—S4: 123.41 (14)  
O4—C44—N6: 122.39 (18)  O8—C94—N12: 122.57 (17)  
O4—C44—C43: 120.97 (17)  O8—C94—C93: 119.92 (17)  
N6—C44—C43: 116.64 (16)  N12—C94—C93: 117.51 (16)  
C46—C45—C50: 119.6 (2)  C96—C95—C100: 117.80 (18)  
C46—C45—N6: 117.1 (2)  C96—C95—N12: 119.36 (18)  
C50—C45—N6: 123.28 (19)  C100—C95—N12: 122.81 (18)  
C47—C46—C45: 119.9 (3)  C95—C96—C97: 120.5 (2)  
C47—C46—H46: 120.1  C95—C96—H96: 119.7  
C45—C46—H46: 120.1  C97—C96—H96: 119.7  
C48—C47—C46: 120.6 (3)  C98—C97—C96: 120.1 (2)  
C48—C47—H47: 119.7  C98—C97—H97: 119.9  
C46—C47—H47: 119.7  C96—C97—H97: 119.9  
C49—C48—C47: 119.4 (2)  C99—C98—C97: 119.6 (2)  
C49—C48—H48: 120.3  C99—C98—H98: 120.2  
C47—C48—H48: 120.3  C97—C98—H98: 120.2  
C48—C49—C50: 121.3 (3)  C98—C99—C100: 121.2 (2)  
C48—C49—H49: 119.3  C98—C99—H99: 119.4  
C50—C49—H49: 119.3  C100—C99—H99: 119.4  
C49—C50—C55—N7: 179.11 (13)  C51—N7—C55—C54: 1.2 (3)  
C5—N1—C1—C2: −1.8 (2)  C55—N7—C51—C52: −177.12 (18)  
C5—N1—C1—C6: 179.72 (16)  C55—N7—C51—C56: −2.7 (3)  
N1—C1—C2—C3: −0.2 (3)  N7—C51—C52—C53: 175.46 (19)  
C6—C1—C2—C3: 178.19 (17)  C56—C51—C52—C53: 177.02 (18)  
N1—C1—C2—C7: −179.46 (16)  C56—C51—C52—C57: −4.8 (3)  
C6—C1—C2—C7: −1.1 (3)  C51—C52—C53—C54: 2.9 (3)  
C1—C2—C3—C4: 2.8 (2)  C57—C52—C53—C54: −176.84 (16)  
C7—C2—C3—C4: −177.93 (15)  C51—C52—C53—C59: −178.19 (17)  
C1—C2—C3—C9: −176.73 (16)  C57—C52—C53—C59: 2.1 (3)  
C7—C2—C3—C9: 2.5 (3)  C57—C52—C53—C59: −1.7 (2)  
C2—C3—C4—C5: −3.4 (2)  C59—C53—C54—C55: 179.43 (17)  
C9—C3—C4—C5: 176.23 (15)  C59—C53—C54—C67: 174.11 (17)  
C2—C3—C4—C17: 175.09 (17)  C52—C53—C54—C67: −4.7 (3)  
C9—C3—C4—C17: −5.3 (3)  C59—C53—C54—C67: 0.0 (3)  
C1—N1—C5—C4: 1.2 (3)  C51—N7—C55—C54: −178.04 (14)  
C1—N1—C5—S1: −179.11 (13)  C51—N7—C55—S3: 0.3 (3)  
C3—C4—C5—N1: 1.5 (3)  C53—C54—C55—N7: 176.41 (17)  
C17—C4—C5—N1: −177.28 (16)  C67—C54—C55—N7: 178.45 (13)  
C3—C4—C5—S1: −178.28 (12)  C53—C54—C55—S3: 1.72 (19)  
C17—C4—C5—S1: 2.97 (18)  C67—C54—C55—S3: −1.41 (14)  
C18—S1—C5—N1: 178.74 (15)  C68—S3—C55—O5: −83.5 (3)  
C18—S1—C5—C4: −1.50 (14)  C68—S3—C55—O5: 96.7 (2)  
C3—C2—C7—O1: 106.6 (2)  C53—C52—C57—O5: −74.2 (2)  
C1—C2—C7—O1: −74.2 (2)  C51—C52—C57—O5: 112.75 (13)  

*Acta Cryst. (2022). E78, 225-230*
| Bond/Ring          | Angle (°) | Bond/Ring          | Angle (°) |
|-------------------|-----------|-------------------|-----------|
| C3—C2—C7—C8      | −76.4 (2) | C53—C52—C57—C58  | 97.7 (2)  |
| C1—C2—C7—C8      | 102.8 (2) | C51—C52—C57—C58  | −82.0 (3) |
| C2—C3—C9—C10     | −53.7 (3) | C52—C53—C59—C60  | 123.5 (2) |
| C4—C3—C9—C10     | 126.8 (2) | C54—C53—C59—C60  | −57.7 (3) |
| C3—C9—C10—C11    | −178.51 (17) | C53—C59—C60—C61 | 179.37 (18) |
| C9—C10—C11—C16   | −18.0 (3) | C59—C60—C61—C62 | −166.9 (2) |
| C9—C10—C11—C12   | 162.22 (19) | C59—C60—C61—C66 | 10.0 (3) |
| C16—C11—C12—C13  | 1.2 (3) | C66—C61—C62—C63 | −1.3 (3) |
| C10—C11—C12—C13  | −178.94 (19) | C60—C61—C62—C63 | 175.8 (2) |
| C11—C12—C13—C14  | −1.1 (3) | C61—C62—C63—C64 | 0.4 (3) |
| C12—C13—C14—C15  | 0.1 (4) | C62—C63—C64—C65 | 0.9 (4) |
| C13—C14—C15—C16  | 0.9 (4) | C63—C64—C65—C66 | −1.3 (4) |
| C14—C15—C16—C11  | −0.7 (3) | C62—C61—C66—C65 | 1.0 (4) |
| C12—C11—C16—C15  | −0.3 (3) | C60—C61—C66—C65 | −176.0 (2) |
| C10—C11—C16—C15  | 179.87 (19) | C64—C65—C66—C61 | 0.3 (4) |
| C5—C4—C17—N2     | 177.33 (16) | C55—C54—C67—N8  | 177.21 (17) |
| C3—C4—C17—N2     | −1.2 (3) | C53—C54—C67—N8  | 1.2 (3) |
| C5—C4—C17—C18    | −3.3 (2) | C55—C54—C67—C68 | −1.1 (2) |
| C3—C4—C17—C18    | 178.22 (17) | C53—C54—C67—C68 | −177.19 (18) |
| N2—C17—C18—C19   | −2.0 (3) | C55—S3—C68—C67  | 0.9 (3) |
| C4—C17—C18—C19   | 178.62 (16) | C54—C67—C68—C69 | 179.30 (15) |
| N2—C17—C18—S1    | −178.41 (14) | N8—C67—C68—S3  | −178.27 (14) |
| C4—C17—C18—S1    | 2.18 (19) | C54—C67—C68—S3  | 0.13 (19) |
| C5—S1—C18—C17    | −0.43 (14) | C55—S3—C68—C67  | 0.71 (14) |
| C5—S1—C18—C19    | −176.87 (15) | C55—S3—C68—C69 | −178.47 (15) |
| C20—N3—C19—O2    | −2.0 (3) | C70—N9—C69—O6   | 6.1 (3) |
| C20—N3—C19—C18   | 177.75 (16) | C70—N9—C69—S3  | −174.07 (16) |
| C17—C18—C19—O2   | 3.5 (3) | C67—C68—C69—O6  | 7.2 (3) |
| S1—C18—C19—O2    | 179.52 (14) | S3—C68—C69—O6  | −173.69 (14) |
| C17—C18—C19—N3   | −176.32 (16) | C67—C68—C69—N9 | −172.62 (16) |
| S1—C18—C19—N3    | −0.3 (2) | S3—C68—C69—N9  | 6.5 (2) |
| C19—N3—C20—C25   | 171.75 (19) | C69—N9—C70—C71 | −44.3 (3) |
| C19—N3—C20—C21   | −9.9 (3) | C69—N9—C70—C75  | 134.98 (19) |
| C25—C20—C21—C22  | −1.0 (3) | C75—C70—C71—C72 | −1.2 (3) |
| N3—C20—C21—C22   | −179.36 (18) | N9—C70—C71—C72 | 178.09 (18) |
| C20—C21—C22—C23  | 0.0 (3) | C70—C71—C72—C73 | 0.1 (3) |
| C21—C22—C23—C24  | 0.5 (3) | C71—C72—C73—C74 | 0.4 (4) |
| C22—C23—C24—C25  | 0.0 (4) | C72—C73—C74—C75 | 0.1 (4) |
| C21—C20—C25—C24  | 1.5 (3) | C73—C74—C75—C70 | −1.2 (4) |
| N3—C20—C25—C24   | 180.0 (2) | C71—C70—C75—C74 | 1.8 (3) |
| C23—C24—C25—C20  | −1.0 (4) | N9—C70—C75—C74 | −177.6 (2) |
| C30—N4—C26—C27   | 1.2 (3) | C80—N10—C76—C81 | 179.18 (19) |
| C30—N4—C26—C31   | −179.6 (2) | C80—N10—C76—C81 | 195.18 (19) |
| N4—C26—C27—C28   | 0.2 (3) | N10—C76—C77—C78 | 0.4 (3) |
| C31—C26—C27—C28  | −179.0 (2) | C81—C76—C77—C78 | 179.5 (2) |
| N4—C26—C27—C32   | −177.7 (2) | N10—C76—C77—C82 | −178.89 (18) |
| C31—C26—C27—C32  | 3.2 (3) | C81—C76—C77—C82 | 1.1 (3) |
| C26—C27—C28—C29  | 0.2 (3) | C76—C77—C78—C79 | 1.9 (3) |
| Bond angles (deg) | | Bond angles (deg) | | Bond angles (deg) |
|------------------|------------------|------------------|
| C32—C27—C28—C29 | 177.97 (18)      | C82—C77—C78—C79 | -179.79 (16) |
| C26—C27—C28—C34 | 179.91 (19)      | C76—C77—C78—C84 | -177.65 (17) |
| C32—C27—C28—C34 | -2.3 (3)         | C82—C77—C78—C84 | 0.7 (3)      |
| C27—C28—C29—C30 | -1.8 (3)         | C77—C78—C79—C80 | -2.7 (2)     |
| C34—C28—C29—C30 | 178.53 (19)      | C84—C78—C79—C80 | 176.80 (16)  |
| C27—C28—C29—C42 | 174.1 (2)        | C77—C78—C79—C92 | 175.63 (18)  |
| C34—C28—C29—C42 | -5.6 (4)         | C84—C78—C79—C92 | -4.8 (3)     |
| C26—N4—C30—C29  | -3.1 (3)         | C76—N10—C80—C79 | 0.8 (3)      |
| C26—N4—C30—S2   | 3.5 (3)          | C76—C77—C80—N10 | 1.5 (3)      |
| C28—C27—C32—O3  | 179.68 (16)      | C92—C79—C80—N10 | -177.16 (17) |
| C26—C27—C32—O3  | -106.0 (2)       | C78—C79—C80—S4  | -178.14 (13) |
| C28—C27—C32—C33 | -104.3 (2)       | C28—C27—C32—C33 | 73.6 (3)     |
| C26—C27—C32—C33 | 128.5 (2)        | C28—C27—C32—C33 | 179.68 (16)  |
| C29—C28—C34—C35 | -51.8 (3)        | C29—C28—C34—C35 | 179.68 (16)  |
| C28—C34—C35—C36 | 170.7 (2)        | C28—C34—C35—C36 | 170.7 (2)    |
| C34—C35—C36—C41 | 178.4 (2)        | C34—C35—C36—C41 | 178.4 (2)    |
| C34—C35—C36—C37 | 2.1 (4)          | C34—C35—C36—C37 | 2.1 (4)      |
| C41—C36—C37—C38 | -1.7 (3)         | C41—C36—C37—C38 | -1.7 (3)     |
| C35—C36—C37—C38 | 174.6 (2)        | C35—C36—C37—C38 | 174.6 (2)    |
| C36—C37—C38—C39 | 0.4 (4)          | C36—C37—C38—C39 | 0.4 (4)      |
| C37—C38—C39—C40 | 1.5 (4)          | C37—C38—C39—C40 | 1.5 (4)      |
| C38—C39—C40—C41 | -2.2 (4)         | C38—C39—C40—C41 | -2.2 (4)     |
| C39—C40—C41—C36 | 1.0 (3)          | C39—C40—C41—C36 | 1.0 (3)      |
| C37—C36—C41—C40 | 1.0 (3)          | C37—C36—C41—C40 | 1.0 (3)      |
| C35—C36—C41—C40 | -175.5 (2)       | C35—C36—C41—C40 | -175.5 (2)   |
| C30—C29—C42—N5  | 176.37 (19)      | C30—C29—C42—N5  | 176.37 (19)  |
| C28—C29—C42—N5  | 0.3 (3)          | C28—C29—C42—N5  | 0.3 (3)      |
| C30—C29—C42—C43 | -2.6 (2)         | C30—C29—C42—C43 | -2.6 (2)     |
| C28—C29—C42—C43 | -178.7 (2)       | C28—C29—C42—C43 | -178.7 (2)   |
| N5—C42—C43—C44  | -3.3 (3)         | N5—C42—C43—C44  | -3.3 (3)     |
| C29—C42—C43—C44 | 175.74 (18)      | C29—C42—C43—C44 | 175.74 (18)  |
| N5—C42—C43—S2   | -178.83 (16)     | N5—C42—C43—S2   | -178.83 (16) |
| C29—C42—C43—N6  | 0.2 (2)          | C29—C42—C43—N6  | 0.2 (2)      |
| C30—S2—C43—C42  | 1.76 (16)        | C30—S2—C43—C42  | 1.76 (16)    |
| C30—S2—C43—C44  | -173.88 (18)     | C30—S2—C43—C44  | -173.88 (18) |
| C45—N6—C44—O4   | -1.5 (3)         | C45—N6—C44—O4   | -1.5 (3)     |
| C45—N6—C44—C43  | 178.27 (19)      | C45—N6—C44—C43  | 178.27 (19)  |
| C42—C43—C44—O4  | 4.3 (3)          | C42—C43—C44—O4  | 4.3 (3)      |
| S2—C43—C44—O4   | 179.46 (17)      | S2—C43—C44—O4   | 179.46 (17)  |
| C42—C43—C44—N6  | -175.42 (19)     | C42—C43—C44—N6  | -175.42 (19) |
| S2—C43—C44—N6   | -0.3 (3)         | S2—C43—C44—N6   | -0.3 (3)     |
C44—N6—C45—C46 158.0 (2) C94—N12—C95—C96 157.0 (2)
C44—N6—C45—C50 −23.3 (3) C94—N12—C95—C100 −25.0 (3)
C50—C45—C46—C47 −0.9 (4) C100—C95—C96—C97 0.0 (3)
N6—C45—C46—C47 177.9 (2) N12—C95—C96—C97 178.1 (2)
C45—C46—C47—C48 0.9 (4) C95—C96—C97—C98 0.3 (4)
C46—C47—C48—C49 0.2 (4) C96—C97—C98—C99 0.2 (4)
C47—C48—C49—C50 −1.3 (4) C97—C98—C99—C100 −0.9 (4)
C48—C49—C50—C45 1.2 (4) C96—C95—C100—C99 −0.8 (3)
C46—C45—C50—C49 −0.1 (3) N12—C95—C100—C99 −178.7 (2)
N6—C45—C50—C49 −178.8 (2) C98—C99—C100—C95 1.2 (4)

**Hydrogen-bond geometry (Å, °)**

Cg8, Cg14 and Cg18 are the centroids of the C36–C41, C70–C75 and C86–C91 benzene rings, respectively.

| D—H···A | D—H | H···A | D···A | D—H···A |
|---------|-----|-------|-------|---------|
| N2—H2A···O2 | 0.91 | 1.98  | 2.703 (2) | 135 |
| N3—H3A···N4i | 0.91 | 2.31  | 3.190 (2) | 164 |
| C8—H8B···Cg14 | 0.98 | 2.67  | 3.537 (2) | 148 |
| C21—H21···O2 | 0.95 | 2.22  | 2.825 (2) | 121 |
| N5—H5A···O4 | 0.91 | 2.03  | 2.717 (2) | 131 |
| N6—H6D···N7ii | 0.91 | 2.38  | 3.231 (2) | 157 |
| C33—H33C···O8iii | 0.98 | 2.47  | 3.411 (3) | 162 |
| C41—H41···Cg18iii | 0.95 | 2.94  | 3.673 (2) | 135 |
| C58—H58B···Cg8iv | 0.98 | 2.91  | 3.534 (3) | 122 |
| C75—H75···S4v | 0.95 | 2.87  | 3.781 (2) | 160 |
| N8—H8D···O6 | 0.91 | 1.98  | 2.701 (2) | 135 |
| N9—H9A···N10ii | 0.91 | 2.22  | 3.106 (2) | 164 |
| N11—H11A···O8 | 0.91 | 1.99  | 2.697 (2) | 134 |
| N12—H12A···N1vi | 0.91 | 2.30  | 3.193 (2) | 168 |

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