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Synthesis, crystal structure and Hirshfeld surface analysis of 1,1′-[oxybis(ethane-2,1-diyl)]bis(2-methylsulfanyl-1*H*-benzo[*d*]imidazole)

Ahmed Moussaif,[a] Lhoussaine El Ghayati,[b] Camille Kalonji Mubengayi,[c] Abdulsalam Alsubari,[d]* El Mokhtar Essassi,[b] Joel T. Mague[e] and Youssef Ramli[f]*

[a]National Center for Nuclear Energy, Science and Technology, Rabat, Morocco, [b]Laboratory of Heterocyclic Organic Chemistry, Medicines Science Research Center, Pharmacochemistry Competence Center, Mohammed V University in Rabat, Faculte des Sciences, Av. Ibn Battouta, BP 1014, Rabat, Morocco, [c]Laboratoire de Chimie et Biochimie, Institut Superieur des Techniques Medicales, Kinshasa, Republique Democratique, Congo, [d]Laboratory of Medicinal Chemistry, Faculty of Clinical Pharmacy, 21 September University, Yemen, [e]Department of Chemistry, Tulane University, New Orleans, LA 70118, USA, and [f]Laboratory of Medicinal Chemistry, Drug Sciences Research Center, Faculty of Medicine and Pharmacy, Mohammed V University in Rabat, Morocco. *Correspondence e-mail: alsubaripharmaco@21umas.edu.ye, y.ramli@um5r.ac.ma

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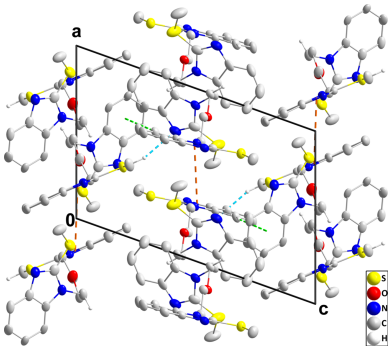
The asymmetric unit of the title compound, $C_{20}H_{22}N_4OS_2$, consists of two independent molecules, one of which is disordered. In each molecule, the mean planes of the terminal benzimidazole moieties are inclined to one another by about 68°. In the crystal, tetramolecular strands are generated by C—H···N hydrogen bonds and C—H···π(ring) interactions and are linked by C—H···π(ring) and π-stacking interactions.

1. Chemical context

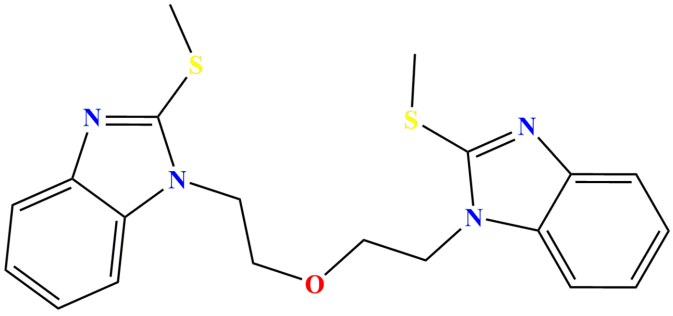
The benzimidazole ring system consists of a five-membered imidazole ring (with two nitrogens included in the heterocyclic structure) fused to another aromatic ring. This structure gives benzimidazoles significant chemical stability and a range of biological properties (Obaid *et al.*, 2022), making them a subject of interest in the pharmacological field.

The benzimidazole ring is a well-known motif recognized for its chemical flexibility, allowing effective interaction with various biological targets. As derivatives of this ring, bis-benzimidazoles share interesting physicochemical properties, such as their ability to interact with biological macromolecules like proteins, enzymes, and DNA. These interactions make them promising candidates for the development of drugs aimed at treating various diseases. Several bisbenzimidazole derivatives have been studied for their activity against various pathogens, including parasites and bacteria. Compounds from this class are used in the treatment of parasitic diseases such as giardiasis, amebiasis, and onchocerciasis. Additionally, some studies have revealed that bisbenzimidazoles possess anti-cancer properties. They work by inhibiting key enzymes in cancer cells, blocking cell division, or inducing mechanisms of programmed cell death (apoptosis). For instance, derivatives like levamisole, used in cancer treatments (Yadav *et al.*, 2018), have shown potential effects in stimulating the immune system and inhibiting tumor growth. Moreover, emerging research suggests that certain bisbenzimidazoles could be beneficial in the treatment of neurodegenerative diseases like Alzheimer's disease (Algul *et al.*, 2025).

Continuing our research in this field (*e.g.* Missioui *et al.*, 2022), we synthesized the title compound 1,1′-[oxybis(ethane-



2,1-diyl)]bis(2-methylsulfanyl-1*H*-benzo[*d*]imidazole) *via* an alkylation reaction. We determined its molecular and crystalline structures, and conducted a Hirshfeld surface analysis to analyze the intermolecular interactions.



2. Structural commentary

The asymmetric unit consists of two independent molecules, one of which is disordered (Figs. 1 and 2). This involves the rotation of one 2-(methylsulfanyl)benzimidazole unit by approximately 170° about the N7—C32 bond in a 0.7200 (13)/0.2800 (13) ratio, while for that at the other end of the molecule a shift of 0.5 Å parallel to the plane of the unit is observed in a 0.775 (6)/0.225 (6) ratio (Fig. 2). In the ordered molecule, the two benzimidazole units are nearly planar as the dihedral angles between their constituent planes are less than 2°, while the dihedral angle between the mean planes of the benzimidazole units in this molecule is 68.38 (9)° (Fig. 1) and the C7—N2—C9 —C10 and the C13—N3—C12—C11 torsion angles are 99.1 (3) and 103.6 (3)°, respectively. In the central chain, the N2—C9—C10—O1 and the C11—O1—C10—C9 torsion angles are, respectively, −179.5 (2) and −180.0 (2)°, while the C10—O1—C11—C12 and the O1—C11—C12—N3 torsion angles are, respectively, 179.9 (2) and −60.0 (3)°. One methylsulfanyl group lies nearly in the plane of the five-membered ring to which it is attached [C8—S1—C7—N1 = −1.8 (3)°], but the other is rotated moderately out of the corresponding plane [C14—S2—C13—N4 = −23.2 (3)°]. The benzimidazole units in the disordered molecule were refined as planar rigid groups and the dihedral angle between their mean planes in the major component is 68.12 (11)° but because of the disorder, comparison of its torsion angles with those of the ordered molecule is not useful. In the ordered molecule, bond distances and interbond angles are as expected for the formulation given.

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

*Cg*1, *Cg*5 and *Cg*11 are the centroids of the N5/C26/C21/N6/C27, the C21-C26 and the C1–C6 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···*Cg*5^{i}	0.95	2.71	3.583 (3)	153
C11—H11*B*···*Cg*11^{ii}	0.99	2.74	3.423 (3)	126
C29—H29*B*···*Cg*1^{iii}	0.99	2.70	3.489 (3)	137
C34—H34*B*···N4^{iv}	0.98	2.50	3.398 (3)	153

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

3. Supramolecular features

In the crystal, the major component of the disordered molecule containing O2 is linked to the molecule containing O1 at $-x+1, -y+2, -z+1$ by a C35—H34*B*···N4 hydrogen bond (Table 1) and this two-molecule unit is linked to its counterpart at $-x+1, -y, -z$ by a C29—H29*B*···*Cg*1 interaction (Table 1 and Fig. 3). These tetramolecular strands are connected by C2—H2···*Cg*5 and C11—H11B···*Cg*11 interactions (Table 1) as well as by π-stacking interactions between inversion-related N1/C6/C1/N2/C7 rings [centroid–centroid distance = 3.6645 (18) Å, dihedral angle = 0.03 (18)°, slippage = 1.06 Å] to generate the full 3-D structure (Fig. 4).

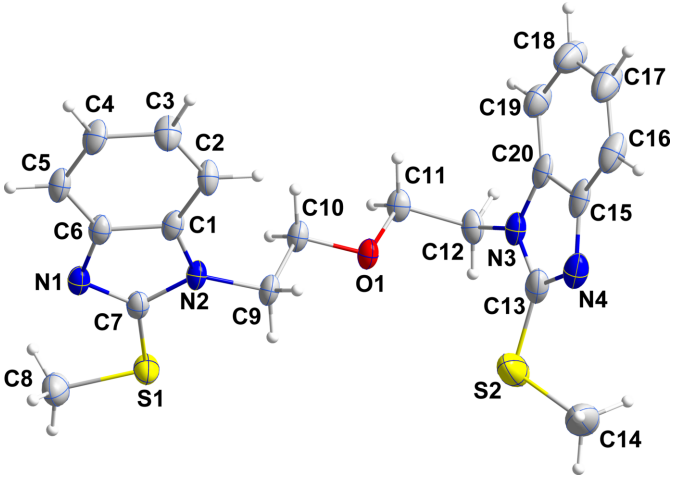


Figure 1
The ordered molecule in the asymmetric unit of the title compound with labeling scheme and 50% probability ellipsoids.

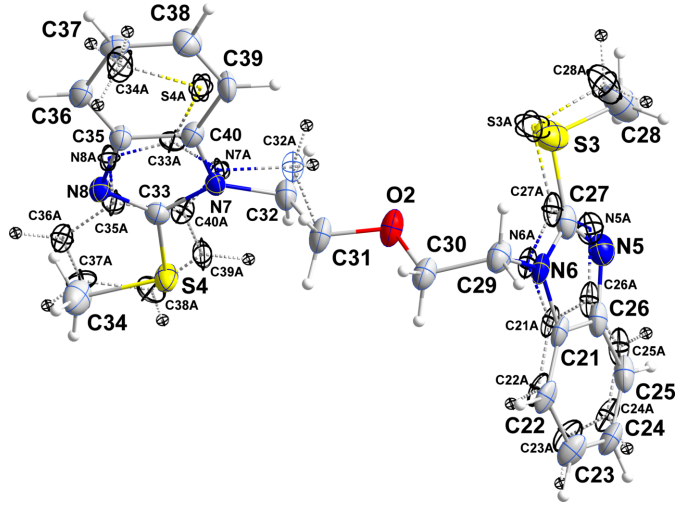


Figure 2
The disordered molecule in the asymmetric unit of the title compound showing the overlay of the two components with the minor component depicted with dashed lines.

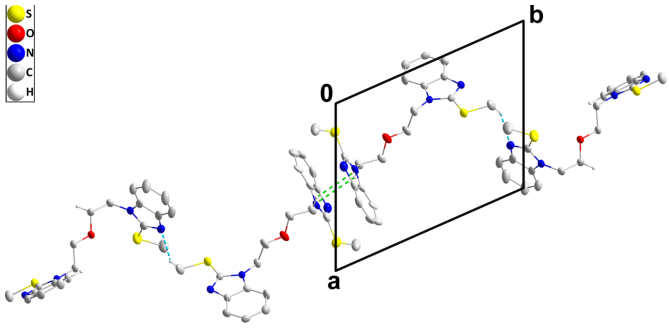


Figure 3
One tetramolecular strand viewed along the *c*-axis direction with C—H···N hydrogen bonds and C—H···π(ring) interactions depicted, respectively, by blue and green dashed lines. Hydrogen atoms not involved in these interactions are omitted for clarity.

4. Database survey

A search of the Cambridge Structural Database (CSD updated to November 2024 (Groom *et al.*, 2016)) with the fragment shown in Fig. 5 (*R* = C) and restricted to only organic compounds generated seven hits. Four of these contained only one 2-(methylsulfanyl)-1*H*-benzamidazole moiety and had *R* = CH_2CH_2OH (DUNZUI: Akonan *et al.*, 2010), 5,6-dihydro-2*H*-pyran-2-one (IHAREP: Hammal *et al.*, 2008), morpholin-4-methyl (SIMCUN: Abou *et al.*, 2007) and the ionic compound 1-methyl-2-(methylsulfanyl)-1*H*-benzimidazol-3-ium iodide (WANXUH: Hasty *et al.*, 2017). For these, the carbon atom of the methysulfanyl group lies in or very close to

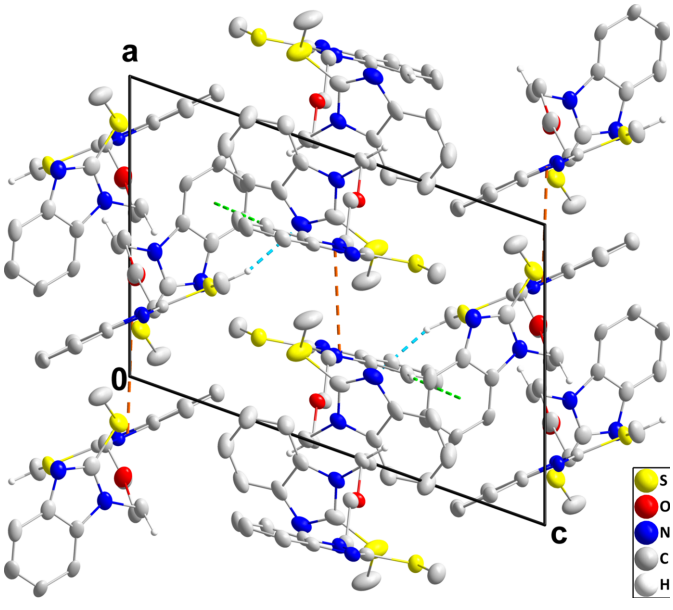


Figure 4
Packing viewed along the *b*-axis direction with C—H···N hydrogen bonds and C—H···π(ring) and π-stacking interactions depicted, respectively, by blue, green and orange dashed lines. Hydrogen atoms not involved in these interactions are omitted for clarity.

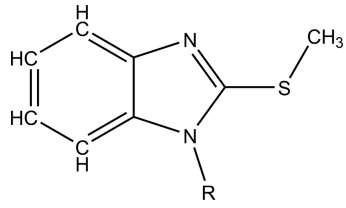


Figure 5
The fragment used for the database search.

the plane of the benzimidazole moiety, while for the first three, the *R* group projects well out of that plane, which is similar to what is seen in the title molecule. In the asymmetric unit of DUNZUI there are two independent molecules and in its crystal packing, there are π-stacking interactions between five-membered rings of one of these. More extensive π-stacking occurs in WANXUH because of its relatively flat steric profile, while in SIMCUN both rings of the benzimidazole moiety participate in π-stacking interactions.

Two of the other examples are more analogous to the title molecule with two 2-(methylsulfanyl)-1*H*-benzamidazole moieties bridged by a $-(CH_2)_3-$ chain (GEVJOH: Yüksektepe *et al.*, 2007) or by a 1,4-$CH_2C_6H_4CH_2$ unit (UGACEM: Rajakannu *et al.*, 2013) while the third has two 3-methyl-2-(methylsulfanyl)-1*H*-benzimidazol-3-ium cations bridged by a 1,3-phenylene group and triflate anions (KEYQUE: Steinke *et al.*, 2023). In GEVJOH, the dihedral angle between the mean planes of the two benzimidazole units is 74.87 (6)° while the torsion angles corresponding to the C7—N2—C9 —C10 and the C13—N3—C12—C11 torsion in the title molecule are, 87.9 (2) and 93.6 (2)°, respectively, similar to the title compound. For the other two, the bridging units are much less flexible with the mean planes of the benzimidazole units in KEYQUE inclined to that of the central phenylene ring by 60.5 (2) and 86.7 (2)°, respectively. UGACEM has crystallographically-imposed centrosymmetry and the unique benzimidazole is essentially perpendicular to the central phenylene ring.

5. Hirshfeld surface analysis

A Hirshfeld surface analysis of the title compound was performed with *CrystalExplorer* (Spackman *et al.*, 2021) to determine the contributions of the several intermolecular interactions in the crystal. Full descriptions of the plots obtained and their interpretations have been published (Tan *et al.*, 2019). The d_{norm} surface for the molecule containing O1 (ordered molecule) calculated over the range −0.1811 to 1.3161 in arbitrary units together with several nearest neighbor molecules including the major component of the disordered molecule is shown in Fig. 6*a*. The C—H···N hydrogen bonds are depicted by red dashed lines and are clearly associated with the dark red spots on the d_{norm} surface. Fig. 6*b* shows the surface for the major component of the disordered molecule calculated over the shape function and showing the characteristic pattern of triangles indicating the presence of the π-stacking interactions (dashed lines) noted in

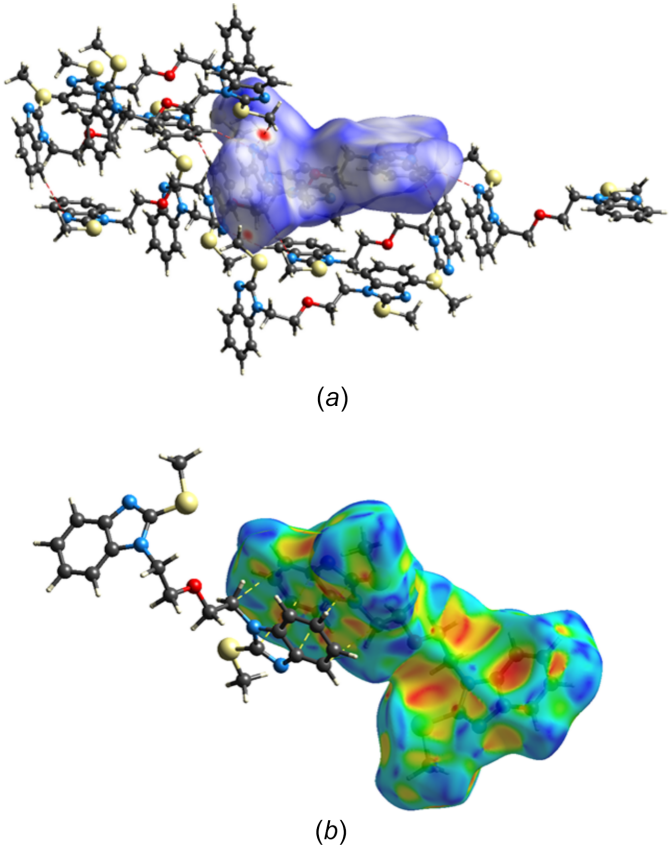


Figure 6
Hirshfeld surfaces: (*a*) the d_{norm} surface for the ordered molecule with several nearest neighbors with C—H···N hydrogen bonds shown as dashed lines; (*b*) the surface calculated over the shape function for the major component of the disordered molecule showing the π-stacking interaction.

Section 3. The 2-D fingerprint plots for all intermolecular interactions and those delineated into specific contacts are presented in Fig. 7. The largest contribution is from H···H contacts (Fig. 7*b*, 52.5% of the total) consistent with the significant hydrogen content of the molecule and the fact that the hydrogen atoms constitute a large portion of its periphery. The next most important contact is C···H/H···C at 21.9% (Fig. 7*c*), which primarily comes from the C—H···π(ring) interactions. The N···H/H···N contacts (Fig. 7*d*), contributing 9.0%, appear as a pair of relatively sharp spikes at $d_e + d_i$ = 2.88 Å and correspond primarily to the C—H···N hydrogen bonds while S···H/H···S contacts (Fig. 7*e*) contribute 8.5%. All other atom···atom contacts contribute a total of 8.1% and are considered quite minor.

6. Synthesis and crystallization

To a 50 mL round-bottom flask, 20 mL of dimethylformamide (DMF) were added followed by the successive addition of 0.0122 moles of 2-methylmercaptobenzimidazole, 0.0150 moles of potassium carbonate (K_2CO_3), 0.0070 moles of 1-chloro-2-(2-chloroethoxy)ethane, and 0.0007 moles of tetrabutylammonium bromide (BTBA). The mixture was stirred at room temperature for 2 h.

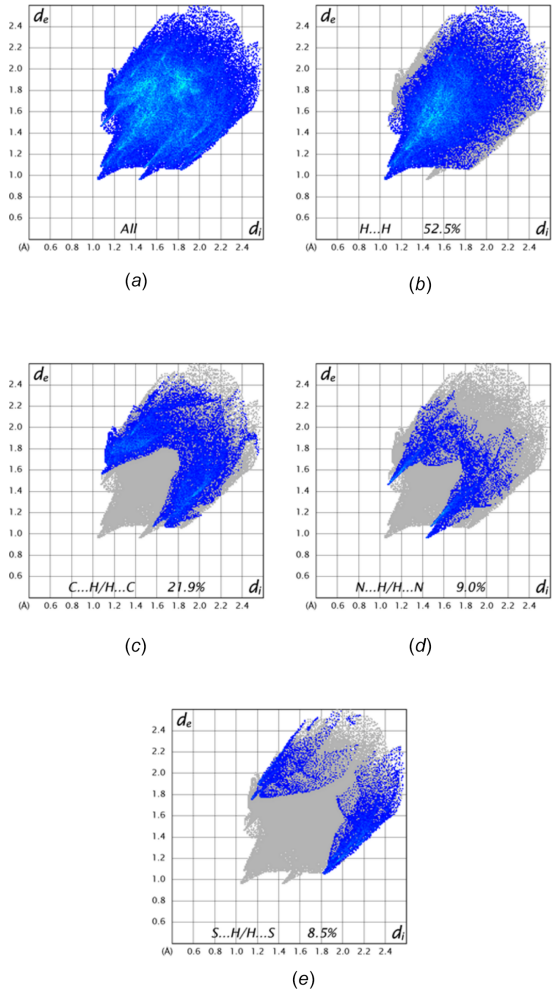


Figure 7
Fingerprint plots showing: (*a*) all intermolecular interactions and those delineated into (*b*) H···H, (*c*) C···H/H···C, (*d*) N···H/H···N and (*e*) S···H/H···S contacts.

The salts were removed by filtration and the solvent was then removed under reduced pressure on a rotary evaporator. The residue obtained was subsequently purified by silica gel column chromatography, using hexane/ethyl acetate (80/20, *v*/*v*) as the mobile phase and recrystallized from ethanol, yielding the title compound with a 72% yield as colorless crystals.

^{1}H NMR (300 MHz, $CDCl_3$) (δ, ppm): 2.54 (*s*, 6H), 3.73 (*t*, ^3J = 7.5 Hz, 4H), 4.33 (*t*, ^{3}J = 7.9 Hz, 4H), 7.48–7.82 (*m*, 8Har).; **^{13}C NMR** (300 MHz, $CDCl_3$) (δ, ppm): 15.5, 49.4, 71.3, 112.7, 124.4, 127.4, 138.8, 148.1, 171.2. **HRMS** (ESI–MS) (*m*/*z*) 398.54.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms attached to carbon were placed in calculated positions (C—H = 0.95–0.99 Å) and included as riding contributions with isotropic displacement parameters 1.2–1.5 times those of the attached atoms. In the molecule containing O2, one end is disordered by a modest

shift in a 0.775 (6)/0.225 (6) ratio while the other end is disordered by an approximate 170° rotation about the C31—C32 bond in a 0.7200 (13)/0.2800 (13) ratio. In both instances, the disordered portions were refined as rigid groups.

Acknowledgements

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Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{20}H_{22}N_4OS_2$
M_r	398.53
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, b, c (Å)	10.6654 (12), 13.5974 (15), 15.7917 (17)
α, β, γ (°)	109.206 (2), 101.687 (2), 107.789 (2)
V (Å^3)	1938.8 (4)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.29
Crystal size (mm)	0.36 × 0.22 × 0.18
Data collection	
Diffractometer	Bruker SMART APEX
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.90, 0.95
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	36334, 10449, 5628
R_{int}	0.074
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.693
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.068, 0.199, 1.00
No. of reflections	10449
No. of parameters	460
No. of restraints	3
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.32, −1.07

Computer programs: *APEX3* and *SAINT* (Bruker, 2015), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2019/1* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

References

Abou, A., Bany, G. E., Kakou-Yao, R., Seikou, T. & Ebby, N. D. (2007). *Acta Cryst.* E**63**, o4218.
Akonan, L., Molou, K. Y. G., Adohi-Krou, A., Abou, A. & Tenon, A. J. (2010). *Acta Cryst.* E**66**, o442.
Algul, O., Mete, B., Turkmenoglu, B., Saglamtas, R., Alagoz, M. A., Dogen, A., Gulcin, I. & Burmaoglu, S. (2025). *J. Mol. Struct.* **1323**, 140800.
Brandenburg, K. & Putz, H. (2012). *DIAMOND* Crystal Impact GbR, Bonn, Germany.
Bruker (2015). *APEX3* and *SAINT*. Bruker AXS LLC, Madison, Wisconsin, USA.
Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.
Hammal, L., Bentarzi, Y., Kaoua, R., Bakhta, S., Nedjar-Kolli, B., Andre, C. & Hoffmann, P. (2008). *J. Soc. Alger. Chim.* **18**, 45–54.
Hasty, S. J., Bandara, M. D., Rath, N. P. & Demchenko, A. V. (2017). *J. Org. Chem.* **82**, 1904–1911.
Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst.* **48**, 3–10.
Missioui, M., Mortada, S., Guerrab, W., Demirtaş, G., Mague, J. T., Ansar, M., El Abbes Faouzi, M., Essassi, E. M., Mehdar, Y. T. H., Aljohani, F. S., Said, M. A. & Ramli, Y. (2022). *Ara. J. Chem.* **15**, 103851.
Obaid, R. J., Mughal, E. U., Naeem, N., Al-Rooqi, M. M., Sadiq, A., Jassas, R. S., Moussa, Z. & Ahmed, S. A. (2022). *Process Biochem.* **120**, 250–259.
Rajakannu, P., Elumalai, P., Mobin, S. M., Lu, K.-L. & Sathiyendiran, M. (2013). *J. Organomet. Chem.* **743**, 17–23.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Spackman, P. R., Turner, M. J., McKinnon, J. J., Wolff, S. K., Grimwood, D. J., Jayatilaka, D. & Spackman, M. A. (2021). *J. Appl. Cryst.* **54**, 1006–1011.
Steinke, T., Engelage, E. & Huber, S. M. (2023). *Acta Cryst.* C**79**, 26–35.
Tan, S. L., Jotani, M. M. & Tiekink, E. R. T. (2019). *Acta Cryst.* E**75**, 308–318.
Yadav, S., Narasimhan, B., Lim, S. M., Ramasamy, K., Vasudevan, M., Shah, S. A. A. & Mathur, A. (2018). *Egypt. J. Basic Appl. Sci.* **5**, 100-109.
Yüksektepe, Ç., Çalışkan, N., Genç, M., Servi, S. & Büyükgüngör, O. (2007). *Acta Cryst.* E**63**, o100–o102.

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Ahmed Moussaif, Lhoussaine El Ghayati, Camille Kalonji Mubengayi, Abdulsalam Alsubari, El Mokhtar Essassi, Joel T. Mague and Youssef Ramli

Computing details

1,1′-[Oxybis(ethane-2,1-diyl)]bis(2-methylsulfanyl-1*H*-benzo[*d*]imidazole)

Crystal data

$C_{20}H_{22}N_4OS_2$
M_r = 398.53
Triclinic, $P\overline{1}$
a = 10.6654 (12) Å
b = 13.5974 (15) Å
c = 15.7917 (17) Å
α = 109.206 (2)°
β = 101.687 (2)°
γ = 107.789 (2)°
V = 1938.8 (4) Å^3
Z = 4
$F(000)$ = 840
D_x = 1.365 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9943 reflections
θ = 2.6–29.0°
μ = 0.29 mm^{-1}
T = 100 K
Column, colourless
0.36 × 0.22 × 0.18 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.3333 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min} = 0.90, T_{max} = 0.95
36334 measured reflections
10449 independent reflections
5628 reflections with $I > 2\sigma(I)$
R_{int} = 0.074
θ_{max} = 29.5°, θ_{min} = 1.7°
h = −14→14
k = −18→18
l = −21→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.199
S = 1.00
10449 reflections
460 parameters
3 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1077P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 1.32 e Å^{-3}
$\Delta\rho_{min}$ = −1.07 e Å^{-3}

Special details

Experimental. The diffraction data were obtained from 3 sets of 400 frames, each of width 0.5 deg. in omega, collected at phi = 0.00, 90.00 and 180.00 deg. and 2 sets of 800 frames, each of width 0.45 deg in phi, collected at omega = -30.00 and 210.00 deg. The scan time was 30 sec/frame.

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 $F^2 > 2\text{sigma}(F^2)$ 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 - 0.99 Å). All were included as riding contributions with isotropic displacement parameters 1.2 - 1.5 times those of the attached atoms. In the molecule containing O2, one end is disordered by a modest shift in a 0.775 (6)/0.225 (6) ratio while the other end is disordered by an approximate 180° rotation about the C31—C32 bond in a 0.7200 (13)/0.2800 (13) ratio. In both instances, the disordered portions were refined as rigid groups.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
S1	0.28306 (8)	0.39883 (6)	0.31081 (5)	0.03271 (19)	
S2	0.28353 (10)	0.94354 (7)	0.40847 (8)	0.0589 (3)	
O1	0.14040 (17)	0.69787 (14)	0.45180 (12)	0.0265 (4)	
N1	0.3274 (2)	0.34561 (18)	0.46399 (16)	0.0261 (5)	
N2	0.3144 (2)	0.51604 (17)	0.49496 (15)	0.0245 (5)	
N3	0.0989 (2)	0.90589 (18)	0.50202 (16)	0.0287 (5)	
N4	0.2898 (2)	1.0698 (2)	0.58629 (18)	0.0370 (6)	
C1	0.3323 (3)	0.5043 (2)	0.57981 (18)	0.0254 (6)	
C2	0.3387 (3)	0.5740 (2)	0.66891 (19)	0.0301 (6)	
H2	0.332501	0.645270	0.681074	0.036*	
C3	0.3544 (3)	0.5346 (2)	0.73914 (19)	0.0347 (7)	
H3	0.358552	0.579523	0.801018	0.042*	
C4	0.3641 (3)	0.4298 (2)	0.7205 (2)	0.0331 (7)	
H4	0.374925	0.405259	0.770283	0.040*	
C5	0.3586 (3)	0.3602 (2)	0.6312 (2)	0.0306 (6)	
H5	0.365884	0.289325	0.619425	0.037*	
C6	0.3419 (3)	0.3990 (2)	0.56012 (19)	0.0256 (6)	
C7	0.3107 (3)	0.4180 (2)	0.42919 (19)	0.0253 (6)	
C8	0.2915 (4)	0.2620 (2)	0.2606 (2)	0.0437 (8)	
H8A	0.210903	0.203462	0.261097	0.066*	
H8B	0.378035	0.264102	0.298536	0.066*	
H8C	0.290012	0.244072	0.194921	0.066*	
C9	0.2979 (3)	0.6119 (2)	0.47908 (19)	0.0266 (6)	
H9A	0.319226	0.612552	0.421047	0.032*	
H9B	0.364700	0.684011	0.533683	0.032*	
C10	0.1505 (3)	0.6037 (2)	0.46773 (19)	0.0269 (6)	
H10A	0.082889	0.531822	0.413204	0.032*	
H10B	0.128798	0.604427	0.525953	0.032*	

C11	0.0038 (3)	0.6962 (2)	0.44035 (19)	0.0277 (6)	
H11A	−0.019845	0.697939	0.498150	0.033*	
H11B	−0.065672	0.625561	0.385448	0.033*	
C12	0.0002 (3)	0.7980 (2)	0.42393 (19)	0.0299 (6)	
H12A	0.021078	0.793568	0.364827	0.036*	
H12B	−0.095464	0.795720	0.414292	0.036*	
C13	0.2245 (3)	0.9775 (2)	0.5057 (2)	0.0360 (7)	
C14	0.3995 (4)	1.0841 (3)	0.4299 (3)	0.0683 (12)	
H14A	0.435052	1.079617	0.376729	0.103*	
H14B	0.478065	1.115441	0.489089	0.103*	
H14C	0.348430	1.133494	0.435353	0.103*	
C15	0.2020 (3)	1.0574 (2)	0.6399 (2)	0.0328 (7)	
C16	0.2183 (3)	1.1275 (2)	0.7317 (2)	0.0410 (8)	
H16	0.298217	1.197014	0.767967	0.049*	
C17	0.1160 (4)	1.0933 (3)	0.7681 (2)	0.0506 (9)	
H17	0.126520	1.139227	0.831367	0.061*	
C18	−0.0043 (4)	0.9924 (3)	0.7150 (2)	0.0517 (9)	
H18	−0.074229	0.972461	0.742407	0.062*	
C19	−0.0230 (3)	0.9218 (2)	0.6238 (2)	0.0384 (7)	
H19	−0.104208	0.853237	0.587287	0.046*	
C20	0.0820 (3)	0.9558 (2)	0.58821 (19)	0.0290 (6)	
O2	0.3432 (2)	0.27334 (17)	0.01613 (14)	0.0388 (5)	
S3	0.16784 (16)	−0.00367 (13)	0.02660 (19)	0.0477 (5)	0.775 (6)
N5	0.3973 (3)	0.04310 (18)	0.17227 (15)	0.0359 (8)	0.775 (6)
N6	0.44458 (15)	0.10270 (18)	0.06022 (10)	0.0285 (6)	0.775 (6)
C21	0.57282 (16)	0.13722 (15)	0.12777 (10)	0.0269 (7)	0.775 (6)
C22	0.70801 (15)	0.1992 (2)	0.13525 (16)	0.0274 (8)	0.775 (6)
H22	0.726802	0.224703	0.088098	0.033*	0.775 (6)
C23	0.81397 (19)	0.2219 (2)	0.21508 (18)	0.0331 (9)	0.775 (6)
H23	0.908138	0.264333	0.223266	0.040*	0.775 (6)
C24	0.7853 (3)	0.1837 (2)	0.28399 (14)	0.0332 (10)	0.775 (6)
H24	0.860720	0.200592	0.337720	0.040*	0.775 (6)
C25	0.6500 (3)	0.1219 (3)	0.27622 (13)	0.0349 (10)	0.775 (6)
H25	0.631661	0.096128	0.323322	0.042*	0.775 (6)
C26	0.5421 (2)	0.09900 (16)	0.19659 (11)	0.0315 (8)	0.775 (6)
C27	0.34510 (18)	0.04853 (11)	0.09217 (12)	0.0343 (8)	0.775 (6)
C28	0.1014 (6)	−0.1083 (4)	0.0703 (4)	0.0574 (16)	0.775 (6)
H28A	−0.000450	−0.147436	0.039998	0.086*	0.775 (6)
H28B	0.143558	−0.163816	0.055384	0.086*	0.775 (6)
H28C	0.124789	−0.070815	0.139505	0.086*	0.775 (6)
S3A	0.1493 (6)	0.0051 (5)	−0.0063 (5)	0.0477 (5)	0.225 (6)
N5A	0.3535 (8)	0.0386 (7)	0.1495 (5)	0.0359 (8)	0.225 (6)
N6A	0.4310 (6)	0.1156 (7)	0.0536 (4)	0.0285 (6)	0.225 (6)
C21A	0.5488 (6)	0.1448 (7)	0.1284 (4)	0.0269 (7)	0.225 (6)
C22A	0.6890 (6)	0.2104 (10)	0.1500 (6)	0.0274 (8)	0.225 (6)
H22A	0.720515	0.243208	0.109577	0.033*	0.225 (6)
C23A	0.7804 (7)	0.2254 (9)	0.2336 (6)	0.0331 (9)	0.225 (6)
H23A	0.877397	0.269824	0.251334	0.040*	0.225 (6)

C24A	0.7330 (9)	0.1763 (10)	0.2925 (5)	0.0332 (10)	0.225 (6)
H24A	0.798933	0.188189	0.349213	0.040*	0.225 (6)
C25A	0.5928 (10)	0.1110 (11)	0.2707 (5)	0.0349 (10)	0.225 (6)
H25A	0.561761	0.077973	0.311061	0.042*	0.225 (6)
C26A	0.4993 (8)	0.0958 (7)	0.1871 (4)	0.0315 (8)	0.225 (6)
C27A	0.3187 (6)	0.0537 (4)	0.0717 (4)	0.0343 (8)	0.225 (6)
C28A	0.067 (2)	−0.1135 (11)	0.0191 (15)	0.0574 (16)	0.225 (6)
H28D	−0.032413	−0.152168	−0.019878	0.086*	0.225 (6)
H28E	0.112093	−0.166856	0.004352	0.086*	0.225 (6)
H28F	0.076253	−0.086085	0.086683	0.086*	0.225 (6)
C29	0.4256 (3)	0.1246 (2)	−0.02772 (19)	0.0342 (7)	
H29A	0.329141	0.074043	−0.072048	0.041*	
H29B	0.490264	0.102472	−0.059150	0.041*	
C30	0.4495 (3)	0.2450 (2)	−0.0135 (2)	0.0330 (6)	
H30A	0.542073	0.298032	0.035349	0.040*	
H30B	0.448728	0.252538	−0.073792	0.040*	
C31	0.3493 (3)	0.3779 (2)	0.0136 (2)	0.0355 (7)	
H31A	0.322927	0.368331	−0.053359	0.043*	
H31B	0.446198	0.436242	0.047735	0.043*	
C32	0.2527 (5)	0.4171 (3)	0.0588 (3)	0.0296 (9)	0.7195 (12)
H32A	0.164360	0.351176	0.040756	0.036*	0.7195 (12)
H32B	0.296278	0.452162	0.128946	0.036*	0.7195 (12)
C32A	0.1981 (13)	0.3781 (6)	0.0241 (9)	0.0296 (9)	0.2805 (12)
H32C	0.119843	0.314492	−0.031603	0.036*	0.2805 (12)
H32D	0.188617	0.368449	0.082266	0.036*	0.2805 (12)
S4	0.39349 (9)	0.68180 (7)	0.19358 (6)	0.0311 (2)	0.7195 (12)
N7	0.22350 (13)	0.49926 (7)	0.02765 (7)	0.0211 (5)	0.7195 (12)
N8	0.21846 (13)	0.66717 (8)	0.03301 (7)	0.0223 (6)	0.7195 (12)
C33	0.27146 (8)	0.61603 (6)	0.07802 (5)	0.0231 (7)	0.7195 (12)
C34	0.41965 (18)	0.82874 (7)	0.22143 (9)	0.0458 (12)	0.7195 (12)
H34A	0.450478	0.850518	0.173404	0.069*	0.7195 (12)
H34B	0.491032	0.878050	0.284386	0.069*	0.7195 (12)
H34C	0.331546	0.836988	0.221551	0.069*	0.7195 (12)
C35	0.12425 (11)	0.57701 (9)	−0.05554 (6)	0.0244 (7)	0.7195 (12)
C36	0.03477 (17)	0.58012 (13)	−0.13155 (8)	0.0288 (8)	0.7195 (12)
H36	0.032523	0.649751	−0.130650	0.035*	0.7195 (12)
C37	−0.04984 (16)	0.47801 (15)	−0.20768 (7)	0.0264 (8)	0.7195 (12)
H37	−0.111558	0.477422	−0.260650	0.032*	0.7195 (12)
C38	−0.04811 (17)	0.37225 (13)	−0.20983 (8)	0.0354 (9)	0.7195 (12)
H38	−0.109548	0.303410	−0.263525	0.042*	0.7195 (12)
C39	0.04091 (19)	0.36846 (10)	−0.13557 (9)	0.0313 (9)	0.7195 (12)
H39	0.043377	0.298685	−0.137039	0.038*	0.7195 (12)
C40	0.12734 (12)	0.47218 (8)	−0.05802 (6)	0.0239 (7)	0.7195 (12)
S4A	0.0421 (3)	0.39830 (19)	−0.15751 (16)	0.0311 (2)	0.2805 (12)
N7A	0.1945 (4)	0.4857 (2)	0.02976 (17)	0.0211 (5)	0.2805 (12)
N8A	0.1597 (4)	0.61691 (18)	−0.02063 (18)	0.0223 (6)	0.2805 (12)
C33A	0.1366 (2)	0.50973 (18)	−0.04389 (15)	0.0231 (7)	0.2805 (12)
C34A	−0.0100 (5)	0.4769 (3)	−0.22092 (19)	0.0458 (12)	0.2805 (12)

H34D	0.073521	0.533118	−0.220876	0.069*	0.2805 (12)
H34E	−0.062280	0.515944	−0.189389	0.069*	0.2805 (12)
H34F	−0.069224	0.424149	−0.286721	0.069*	0.2805 (12)
C35A	0.2426 (3)	0.6713 (2)	0.07740 (18)	0.0244 (7)	0.2805 (12)
C36A	0.3022 (5)	0.7864 (2)	0.1396 (2)	0.0288 (8)	0.2805 (12)
H36A	0.287487	0.841980	0.119762	0.035*	0.2805 (12)
C37A	0.3831 (5)	0.8157 (3)	0.2307 (2)	0.0264 (8)	0.2805 (12)
H37A	0.424704	0.893413	0.274827	0.032*	0.2805 (12)
C38A	0.4068 (5)	0.7329 (4)	0.26154 (19)	0.0354 (9)	0.2805 (12)
H38A	0.464784	0.757051	0.324994	0.042*	0.2805 (12)
C39A	0.3472 (6)	0.6189 (3)	0.20094 (18)	0.0313 (9)	0.2805 (12)
H39A	0.361568	0.563534	0.221265	0.038*	0.2805 (12)
C40A	0.2647 (4)	0.5887 (2)	0.10817 (16)	0.0239 (7)	0.2805 (12)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0413 (4)	0.0294 (4)	0.0308 (4)	0.0179 (3)	0.0115 (3)	0.0135 (3)
S2	0.0604 (6)	0.0366 (5)	0.0818 (7)	0.0194 (4)	0.0425 (5)	0.0165 (5)
O1	0.0267 (9)	0.0217 (9)	0.0318 (10)	0.0118 (8)	0.0049 (8)	0.0130 (8)
N1	0.0244 (11)	0.0220 (11)	0.0314 (12)	0.0103 (9)	0.0060 (9)	0.0117 (10)
N2	0.0258 (11)	0.0195 (11)	0.0274 (12)	0.0105 (9)	0.0036 (9)	0.0108 (9)
N3	0.0279 (12)	0.0205 (11)	0.0346 (13)	0.0108 (9)	0.0022 (10)	0.0118 (10)
N4	0.0293 (13)	0.0271 (13)	0.0509 (16)	0.0102 (10)	0.0052 (12)	0.0180 (12)
C1	0.0237 (13)	0.0214 (13)	0.0272 (14)	0.0074 (11)	0.0013 (11)	0.0117 (11)
C2	0.0361 (15)	0.0189 (13)	0.0272 (14)	0.0122 (11)	−0.0003 (12)	0.0056 (11)
C3	0.0446 (17)	0.0294 (15)	0.0226 (14)	0.0157 (13)	0.0009 (12)	0.0074 (12)
C4	0.0398 (16)	0.0295 (15)	0.0294 (15)	0.0150 (13)	0.0016 (12)	0.0167 (13)
C5	0.0317 (14)	0.0225 (13)	0.0345 (16)	0.0112 (11)	0.0023 (12)	0.0133 (12)
C6	0.0221 (13)	0.0219 (13)	0.0296 (14)	0.0083 (11)	0.0029 (11)	0.0109 (11)
C7	0.0225 (13)	0.0220 (13)	0.0306 (14)	0.0098 (11)	0.0064 (11)	0.0111 (11)
C8	0.060 (2)	0.0313 (16)	0.0424 (18)	0.0206 (15)	0.0217 (16)	0.0134 (15)
C9	0.0303 (14)	0.0197 (13)	0.0306 (14)	0.0112 (11)	0.0059 (11)	0.0130 (11)
C10	0.0294 (14)	0.0190 (12)	0.0308 (14)	0.0100 (11)	0.0050 (11)	0.0115 (11)
C11	0.0256 (13)	0.0232 (13)	0.0278 (14)	0.0094 (11)	−0.0004 (11)	0.0091 (11)
C12	0.0292 (14)	0.0244 (14)	0.0304 (15)	0.0134 (11)	0.0000 (11)	0.0085 (12)
C13	0.0309 (15)	0.0252 (15)	0.0519 (19)	0.0127 (12)	0.0090 (14)	0.0177 (14)
C14	0.070 (3)	0.043 (2)	0.107 (3)	0.0210 (19)	0.059 (3)	0.033 (2)
C15	0.0362 (15)	0.0224 (14)	0.0328 (15)	0.0101 (12)	−0.0059 (12)	0.0151 (12)
C16	0.0485 (19)	0.0257 (15)	0.0320 (16)	0.0055 (13)	−0.0047 (14)	0.0122 (13)
C17	0.080 (3)	0.0287 (16)	0.0340 (17)	0.0131 (17)	0.0156 (17)	0.0123 (14)
C18	0.072 (2)	0.0325 (17)	0.044 (2)	0.0095 (17)	0.0270 (18)	0.0151 (16)
C19	0.0450 (18)	0.0246 (15)	0.0377 (17)	0.0072 (13)	0.0098 (14)	0.0128 (13)
C20	0.0314 (14)	0.0215 (13)	0.0326 (15)	0.0105 (11)	−0.0001 (12)	0.0161 (12)
O2	0.0555 (13)	0.0383 (12)	0.0400 (12)	0.0330 (11)	0.0195 (10)	0.0219 (10)
S3	0.0413 (6)	0.0394 (6)	0.0431 (11)	0.0092 (5)	0.0076 (7)	0.0051 (7)
N5	0.044 (2)	0.0291 (14)	0.0327 (19)	0.0147 (16)	0.0109 (17)	0.0124 (14)
N6	0.0403 (14)	0.0231 (13)	0.0288 (13)	0.0213 (11)	0.0092 (11)	0.0122 (11)

C21	0.0387 (18)	0.0241 (14)	0.0267 (14)	0.0242 (14)	0.0103 (13)	0.0107 (12)
C22	0.0408 (18)	0.0338 (17)	0.0217 (16)	0.0308 (15)	0.0161 (13)	0.0103 (14)
C23	0.040 (2)	0.0467 (19)	0.0254 (19)	0.0306 (17)	0.0174 (15)	0.0143 (16)
C24	0.042 (3)	0.0400 (19)	0.0301 (17)	0.031 (2)	0.0099 (17)	0.0170 (15)
C25	0.060 (3)	0.0230 (17)	0.0246 (16)	0.023 (2)	0.0099 (19)	0.0104 (14)
C26	0.050 (3)	0.0226 (15)	0.0291 (17)	0.0231 (17)	0.0136 (17)	0.0116 (13)
C27	0.047 (2)	0.0216 (15)	0.037 (2)	0.0199 (15)	0.0151 (17)	0.0095 (15)
C28	0.060 (3)	0.036 (2)	0.071 (4)	0.014 (2)	0.041 (3)	0.011 (3)
S3A	0.0413 (6)	0.0394 (6)	0.0431 (11)	0.0092 (5)	0.0076 (7)	0.0051 (7)
N5A	0.044 (2)	0.0291 (14)	0.0327 (19)	0.0147 (16)	0.0109 (17)	0.0124 (14)
N6A	0.0403 (14)	0.0231 (13)	0.0288 (13)	0.0213 (11)	0.0092 (11)	0.0122 (11)
C21A	0.0387 (18)	0.0241 (14)	0.0267 (14)	0.0242 (14)	0.0103 (13)	0.0107 (12)
C22A	0.0408 (18)	0.0338 (17)	0.0217 (16)	0.0308 (15)	0.0161 (13)	0.0103 (14)
C23A	0.040 (2)	0.0467 (19)	0.0254 (19)	0.0306 (17)	0.0174 (15)	0.0143 (16)
C24A	0.042 (3)	0.0400 (19)	0.0301 (17)	0.031 (2)	0.0099 (17)	0.0170 (15)
C25A	0.060 (3)	0.0230 (17)	0.0246 (16)	0.023 (2)	0.0099 (19)	0.0104 (14)
C26A	0.050 (3)	0.0226 (15)	0.0291 (17)	0.0231 (17)	0.0136 (17)	0.0116 (13)
C27A	0.047 (2)	0.0216 (15)	0.037 (2)	0.0199 (15)	0.0151 (17)	0.0095 (15)
C28A	0.060 (3)	0.036 (2)	0.071 (4)	0.014 (2)	0.041 (3)	0.011 (3)
C29	0.0439 (17)	0.0308 (15)	0.0270 (15)	0.0225 (13)	0.0063 (13)	0.0076 (12)
C30	0.0437 (17)	0.0322 (15)	0.0267 (15)	0.0243 (13)	0.0080 (13)	0.0105 (12)
C31	0.0514 (18)	0.0339 (16)	0.0346 (16)	0.0293 (14)	0.0152 (14)	0.0186 (14)
C32	0.041 (3)	0.023 (2)	0.027 (3)	0.016 (2)	0.0091 (19)	0.0118 (19)
C32A	0.041 (3)	0.023 (2)	0.027 (3)	0.016 (2)	0.0091 (19)	0.0118 (19)
S4	0.0366 (5)	0.0262 (5)	0.0259 (5)	0.0137 (4)	0.0005 (4)	0.0104 (4)
N7	0.0230 (14)	0.0191 (12)	0.0247 (12)	0.0087 (10)	0.0093 (10)	0.0120 (10)
N8	0.0272 (17)	0.0227 (16)	0.0187 (16)	0.0118 (13)	0.0055 (12)	0.0102 (13)
C33	0.0222 (17)	0.0232 (17)	0.0217 (17)	0.0077 (14)	0.0074 (13)	0.0083 (14)
C34	0.054 (3)	0.033 (2)	0.036 (2)	0.024 (2)	0.003 (2)	0.0001 (19)
C35	0.0278 (18)	0.0218 (17)	0.0227 (19)	0.0111 (15)	0.0054 (15)	0.0092 (15)
C36	0.0316 (19)	0.0306 (19)	0.0287 (19)	0.0161 (16)	0.0084 (15)	0.0154 (16)
C37	0.0229 (17)	0.035 (2)	0.0168 (17)	0.0100 (15)	0.0023 (14)	0.0100 (16)
C38	0.036 (2)	0.031 (2)	0.029 (2)	0.0118 (17)	0.0061 (17)	0.0058 (17)
C39	0.043 (2)	0.0206 (18)	0.033 (2)	0.0149 (17)	0.0077 (17)	0.0149 (16)
C40	0.0272 (18)	0.0255 (18)	0.0216 (17)	0.0146 (15)	0.0075 (14)	0.0099 (14)
S4A	0.0366 (5)	0.0262 (5)	0.0259 (5)	0.0137 (4)	0.0005 (4)	0.0104 (4)
N7A	0.0230 (14)	0.0191 (12)	0.0247 (12)	0.0087 (10)	0.0093 (10)	0.0120 (10)
N8A	0.0272 (17)	0.0227 (16)	0.0187 (16)	0.0118 (13)	0.0055 (12)	0.0102 (13)
C33A	0.0222 (17)	0.0232 (17)	0.0217 (17)	0.0077 (14)	0.0074 (13)	0.0083 (14)
C34A	0.054 (3)	0.033 (2)	0.036 (2)	0.024 (2)	0.003 (2)	0.0001 (19)
C35A	0.0278 (18)	0.0218 (17)	0.0227 (19)	0.0111 (15)	0.0054 (15)	0.0092 (15)
C36A	0.0316 (19)	0.0306 (19)	0.0287 (19)	0.0161 (16)	0.0084 (15)	0.0154 (16)
C37A	0.0229 (17)	0.035 (2)	0.0168 (17)	0.0100 (15)	0.0023 (14)	0.0100 (16)
C38A	0.036 (2)	0.031 (2)	0.029 (2)	0.0118 (17)	0.0061 (17)	0.0058 (17)
C39A	0.043 (2)	0.0206 (18)	0.033 (2)	0.0149 (17)	0.0077 (17)	0.0149 (16)
C40A	0.0272 (18)	0.0255 (18)	0.0216 (17)	0.0146 (15)	0.0075 (14)	0.0099 (14)

Geometric parameters (Å, º)

S1—C7	1.749 (3)	S3A—C27A	1.7474
S1—C8	1.805 (3)	S3A—C28A	1.799 (5)
S2—C13	1.753 (3)	N5A—C27A	1.3103
S2—C14	1.805 (3)	N5A—C26A	1.3998
O1—C10	1.414 (3)	N6A—C29	1.321 (6)
O1—C11	1.423 (3)	N6A—C27A	1.3808
N1—C7	1.314 (3)	N6A—C21A	1.3843
N1—C6	1.402 (3)	C21A—C22A	1.3879
N2—C7	1.377 (3)	C21A—C26A	1.4038
N2—C1	1.383 (3)	C22A—C23A	1.3840
N2—C9	1.460 (3)	C22A—H22A	0.9500
N3—C13	1.371 (4)	C23A—C24A	1.3994
N3—C20	1.383 (4)	C23A—H23A	0.9500
N3—C12	1.457 (3)	C24A—C25A	1.3863
N4—C13	1.317 (4)	C24A—H24A	0.9500
N4—C15	1.393 (4)	C25A—C26A	1.3929
C1—C2	1.388 (4)	C25A—H25A	0.9500
C1—C6	1.402 (3)	C28A—H28D	0.9800
C2—C3	1.383 (4)	C28A—H28E	0.9800
C2—H2	0.9500	C28A—H28F	0.9800
C3—C4	1.399 (4)	C29—C30	1.508 (4)
C3—H3	0.9500	C29—H29A	0.9900
C4—C5	1.392 (4)	C29—H29B	0.9900
C4—H4	0.9500	C30—H30A	0.9900
C5—C6	1.392 (4)	C30—H30B	0.9900
C5—H5	0.9500	C31—C32	1.495 (5)
C8—H8A	0.9800	C31—C32A	1.654 (13)
C8—H8B	0.9800	C31—H31A	0.9900
C8—H8C	0.9800	C31—H31B	0.9900
C9—C10	1.511 (4)	C32—N7	1.449 (3)
C9—H9A	0.9900	C32—H32A	0.9900
C9—H9B	0.9900	C32—H32B	0.9900
C10—H10A	0.9900	C32A—N7A	1.449 (4)
C10—H10B	0.9900	C32A—H32C	0.9900
C11—C12	1.500 (3)	C32A—H32D	0.9900
C11—H11A	0.9900	S4—C33	1.7540
C11—H11B	0.9900	S4—C34	1.8152
C12—H12A	0.9900	N7—C40	1.3773
C12—H12B	0.9900	N7—C33	1.3868
C14—H14A	0.9800	N8—C33	1.3081
C14—H14B	0.9800	N8—C35	1.4206
C14—H14C	0.9800	C34—H34A	0.9800
C15—C16	1.388 (4)	C34—H34B	0.9800
C15—C20	1.402 (4)	C34—H34C	0.9800
C16—C17	1.363 (5)	C35—C36	1.3954
C16—H16	0.9500	C35—C40	1.4237

C17—C18	1.401 (4)	C36—C37	1.3726
C17—H17	0.9500	C36—H36	0.9500
C18—C19	1.375 (4)	C37—C38	1.4330
C18—H18	0.9500	C37—H37	0.9500
C19—C20	1.376 (4)	C38—C39	1.3777
C19—H19	0.9500	C38—H38	0.9500
O2—C31	1.418 (3)	C39—C40	1.3966
O2—C30	1.420 (3)	C39—H39	0.9500
S3—C27	1.7474	S4A—C33A	1.7540
S3—C28	1.798 (5)	S4A—C34A	1.8152
N5—C27	1.3103	N7A—C40A	1.3773
N5—C26	1.3998	N7A—C33A	1.3867
N6—C27	1.3808	N8A—C33A	1.3081
N6—C21	1.3843	N8A—C35A	1.4206
N6—C29	1.501 (3)	C34A—H34D	0.9800
C21—C22	1.3879	C34A—H34E	0.9800
C21—C26	1.4038	C34A—H34F	0.9800
C22—C23	1.3839	C35A—C36A	1.3954
C22—H22	0.9500	C35A—C40A	1.4237
C23—C24	1.3994	C36A—C37A	1.3726
C23—H23	0.9500	C36A—H36A	0.9500
C24—C25	1.3863	C37A—C38A	1.4330
C24—H24	0.9500	C37A—H37A	0.9500
C25—C26	1.3930	C38A—C39A	1.3776
C25—H25	0.9500	C38A—H38A	0.9500
C28—H28A	0.9800	C39A—C40A	1.3966
C28—H28B	0.9800	C39A—H39A	0.9500
C28—H28C	0.9800		

C7—S1—C8	100.14 (14)	C29—N6A—C21A	127.8 (3)
C13—S2—C14	99.88 (16)	C27A—N6A—C21A	106.1
C10—O1—C11	111.49 (18)	N6A—C21A—C22A	131.6
C7—N1—C6	103.9 (2)	N6A—C21A—C26A	105.4
C7—N2—C1	106.1 (2)	C22A—C21A—C26A	123.0
C7—N2—C9	127.7 (2)	C23A—C22A—C21A	116.4
C1—N2—C9	126.2 (2)	C23A—C22A—H22A	121.8
C13—N3—C20	106.6 (2)	C21A—C22A—H22A	121.8
C13—N3—C12	127.9 (3)	C22A—C23A—C24A	121.4
C20—N3—C12	125.5 (2)	C22A—C23A—H23A	119.3
C13—N4—C15	104.2 (2)	C24A—C23A—H23A	119.3
N2—C1—C2	131.7 (2)	C25A—C24A—C23A	122.0
N2—C1—C6	105.5 (2)	C25A—C24A—H24A	119.0
C2—C1—C6	122.7 (2)	C23A—C24A—H24A	119.0
C3—C2—C1	116.8 (2)	C24A—C25A—C26A	117.4
C3—C2—H2	121.6	C24A—C25A—H25A	121.3
C1—C2—H2	121.6	C26A—C25A—H25A	121.3
C2—C3—C4	121.0 (3)	C25A—C26A—N5A	129.7
C2—C3—H3	119.5	C25A—C26A—C21A	119.9

C4—C3—H3	119.5	N5A—C26A—C21A	110.3
C5—C4—C3	122.1 (3)	N5A—C27A—N6A	114.0
C5—C4—H4	118.9	N5A—C27A—S3A	126.5
C3—C4—H4	118.9	N6A—C27A—S3A	119.5
C6—C5—C4	117.1 (2)	S3A—C28A—H28D	109.5
C6—C5—H5	121.5	S3A—C28A—H28E	109.5
C4—C5—H5	121.5	H28D—C28A—H28E	109.5
C5—C6—C1	120.2 (2)	S3A—C28A—H28F	109.5
C5—C6—N1	129.4 (2)	H28D—C28A—H28F	109.5
C1—C6—N1	110.3 (2)	H28E—C28A—H28F	109.5
N1—C7—N2	114.2 (2)	N6A—C29—C30	109.5 (4)
N1—C7—S1	126.1 (2)	N6—C29—C30	116.4 (2)
N2—C7—S1	119.69 (19)	N6—C29—H29A	108.2
S1—C8—H8A	109.5	C30—C29—H29A	108.2
S1—C8—H8B	109.5	N6—C29—H29B	108.2
H8A—C8—H8B	109.5	C30—C29—H29B	108.2
S1—C8—H8C	109.5	H29A—C29—H29B	107.3
H8A—C8—H8C	109.5	O2—C30—C29	110.0 (2)
H8B—C8—H8C	109.5	O2—C30—H30A	109.7
N2—C9—C10	110.6 (2)	C29—C30—H30A	109.7
N2—C9—H9A	109.5	O2—C30—H30B	109.7
C10—C9—H9A	109.5	C29—C30—H30B	109.7
N2—C9—H9B	109.5	H30A—C30—H30B	108.2
C10—C9—H9B	109.5	O2—C31—C32	110.8 (2)
H9A—C9—H9B	108.1	O2—C31—C32A	102.3 (3)
O1—C10—C9	108.1 (2)	O2—C31—H31A	109.5
O1—C10—H10A	110.1	C32—C31—H31A	109.5
C9—C10—H10A	110.1	O2—C31—H31B	109.5
O1—C10—H10B	110.1	C32—C31—H31B	109.5
C9—C10—H10B	110.1	H31A—C31—H31B	108.1
H10A—C10—H10B	108.4	N7—C32—C31	109.8 (3)
O1—C11—C12	108.8 (2)	N7—C32—H32A	109.7
O1—C11—H11A	109.9	C31—C32—H32A	109.7
C12—C11—H11A	109.9	N7—C32—H32B	109.7
O1—C11—H11B	109.9	C31—C32—H32B	109.7
C12—C11—H11B	109.9	H32A—C32—H32B	108.2
H11A—C11—H11B	108.3	N7A—C32A—C31	108.3 (7)
N3—C12—C11	113.5 (2)	N7A—C32A—H32C	110.0
N3—C12—H12A	108.9	C31—C32A—H32C	110.0
C11—C12—H12A	108.9	N7A—C32A—H32D	110.0
N3—C12—H12B	108.9	C31—C32A—H32D	110.0
C11—C12—H12B	108.9	H32C—C32A—H32D	108.4
H12A—C12—H12B	107.7	C33—S4—C34	99.7
N4—C13—N3	113.6 (3)	C40—N7—C33	105.9
N4—C13—S2	126.0 (2)	C40—N7—C32	124.77 (17)
N3—C13—S2	120.4 (2)	C33—N7—C32	129.05 (17)
S2—C14—H14A	109.5	C33—N8—C35	103.7
S2—C14—H14B	109.5	N8—C33—N7	115.1

H14A—C14—H14B	109.5	N8—C33—S4	125.9
S2—C14—H14C	109.5	N7—C33—S4	119.0
H14A—C14—H14C	109.5	S4—C34—H34A	109.5
H14B—C14—H14C	109.5	S4—C34—H34B	109.5
C16—C15—N4	130.1 (3)	H34A—C34—H34B	109.5
C16—C15—C20	119.5 (3)	S4—C34—H34C	109.5
N4—C15—C20	110.5 (3)	H34A—C34—H34C	109.5
C17—C16—C15	117.9 (3)	H34B—C34—H34C	109.5
C17—C16—H16	121.1	C36—C35—N8	129.5
C15—C16—H16	121.1	C36—C35—C40	121.0
C16—C17—C18	122.0 (3)	N8—C35—C40	109.5
C16—C17—H17	119.0	C37—C36—C35	117.0
C18—C17—H17	119.0	C37—C36—H36	121.5
C19—C18—C17	121.2 (3)	C35—C36—H36	121.5
C19—C18—H18	119.4	C36—C37—C38	122.1
C17—C18—H18	119.4	C36—C37—H37	118.9
C18—C19—C20	116.5 (3)	C38—C37—H37	118.9
C18—C19—H19	121.8	C39—C38—C37	121.3
C20—C19—H19	121.8	C39—C38—H38	119.4
C19—C20—N3	131.9 (2)	C37—C38—H38	119.4
C19—C20—C15	123.0 (3)	C38—C39—C40	116.8
N3—C20—C15	105.1 (2)	C38—C39—H39	121.6
C31—O2—C30	110.7 (2)	C40—C39—H39	121.6
C27—S3—C28	98.26 (19)	N7—C40—C39	132.2
C27—N5—C26	104.2	N7—C40—C35	105.9
C27—N6—C21	106.1	C39—C40—C35	121.8
C27—N6—C29	129.48 (13)	C33A—S4A—C34A	99.7
C21—N6—C29	124.46 (13)	C40A—N7A—C33A	105.9
N6—C21—C22	131.6	C40A—N7A—C32A	125.9 (5)
N6—C21—C26	105.4	C33A—N7A—C32A	127.7 (5)
C22—C21—C26	123.0	C33A—N8A—C35A	103.7
C23—C22—C21	116.4	N8A—C33A—N7A	115.1
C23—C22—H22	121.8	N8A—C33A—S4A	125.9
C21—C22—H22	121.8	N7A—C33A—S4A	119.0
C22—C23—C24	121.4	S4A—C34A—H34D	109.5
C22—C23—H23	119.3	S4A—C34A—H34E	109.5
C24—C23—H23	119.3	H34D—C34A—H34E	109.5
C25—C24—C23	122.0	S4A—C34A—H34F	109.5
C25—C24—H24	119.0	H34D—C34A—H34F	109.5
C23—C24—H24	119.0	H34E—C34A—H34F	109.5
C24—C25—C26	117.4	C36A—C35A—N8A	129.5
C24—C25—H25	121.3	C36A—C35A—C40A	121.0
C26—C25—H25	121.3	N8A—C35A—C40A	109.5
C25—C26—N5	129.7	C37A—C36A—C35A	117.0
C25—C26—C21	119.9	C37A—C36A—H36A	121.5
N5—C26—C21	110.3	C35A—C36A—H36A	121.5
N5—C27—N6	114.0	C36A—C37A—C38A	122.1
N5—C27—S3	126.5	C36A—C37A—H37A	118.9

N6—C27—S3	119.5	C38A—C37A—H37A	118.9
S3—C28—H28A	109.5	C39A—C38A—C37A	121.3
S3—C28—H28B	109.5	C39A—C38A—H38A	119.4
H28A—C28—H28B	109.5	C37A—C38A—H38A	119.4
S3—C28—H28C	109.5	C38A—C39A—C40A	116.8
H28A—C28—H28C	109.5	C38A—C39A—H39A	121.6
H28B—C28—H28C	109.5	C40A—C39A—H39A	121.6
C27A—S3A—C28A	98.3 (8)	N7A—C40A—C39A	132.2
C27A—N5A—C26A	104.2	N7A—C40A—C35A	105.9
C29—N6A—C27A	125.0 (3)	C39A—C40A—C35A	121.8

C7—N2—C1—C2	−177.5 (3)	N6A—C21A—C22A—C23A	178.1
C9—N2—C1—C2	0.5 (4)	C26A—C21A—C22A—C23A	0.3
C7—N2—C1—C6	1.4 (3)	C21A—C22A—C23A—C24A	0.2
C9—N2—C1—C6	179.4 (2)	C22A—C23A—C24A—C25A	−0.3
N2—C1—C2—C3	178.4 (3)	C23A—C24A—C25A—C26A	−0.2
C6—C1—C2—C3	−0.3 (4)	C24A—C25A—C26A—N5A	−177.3
C1—C2—C3—C4	0.4 (4)	C24A—C25A—C26A—C21A	0.7
C2—C3—C4—C5	0.0 (4)	C27A—N5A—C26A—C25A	178.0
C3—C4—C5—C6	−0.4 (4)	C27A—N5A—C26A—C21A	−0.1
C4—C5—C6—C1	0.4 (4)	N6A—C21A—C26A—C25A	−179.0
C4—C5—C6—N1	−177.2 (3)	C22A—C21A—C26A—C25A	−0.8
N2—C1—C6—C5	−179.1 (2)	N6A—C21A—C26A—N5A	−0.7
C2—C1—C6—C5	−0.1 (4)	C22A—C21A—C26A—N5A	177.6
N2—C1—C6—N1	−1.1 (3)	C26A—N5A—C27A—N6A	0.9
C2—C1—C6—N1	177.9 (2)	C26A—N5A—C27A—S3A	−178.4
C7—N1—C6—C5	178.1 (3)	C29—N6A—C27A—N5A	167.2 (9)
C7—N1—C6—C1	0.3 (3)	C21A—N6A—C27A—N5A	−1.3
C6—N1—C7—N2	0.7 (3)	C29—N6A—C27A—S3A	−13.5 (9)
C6—N1—C7—S1	−178.45 (19)	C21A—N6A—C27A—S3A	178.0
C1—N2—C7—N1	−1.4 (3)	C28A—S3A—C27A—N5A	−25.4 (8)
C9—N2—C7—N1	−179.3 (2)	C28A—S3A—C27A—N6A	155.3 (8)
C1—N2—C7—S1	177.80 (17)	C27A—N6A—C29—C30	112.2 (6)
C9—N2—C7—S1	−0.1 (3)	C21A—N6A—C29—C30	−81.8 (5)
C8—S1—C7—N1	−1.8 (3)	C27—N6—C29—C30	105.3 (3)
C8—S1—C7—N2	179.1 (2)	C21—N6—C29—C30	−73.6 (3)
C7—N2—C9—C10	99.1 (3)	C31—O2—C30—C29	−169.6 (2)
C1—N2—C9—C10	−78.4 (3)	N6A—C29—C30—O2	−61.3 (4)
C11—O1—C10—C9	−180.0 (2)	N6—C29—C30—O2	−68.0 (3)
N2—C9—C10—O1	−179.5 (2)	C30—O2—C31—C32	−171.2 (3)
C10—O1—C11—C12	179.9 (2)	C30—O2—C31—C32A	166.8 (5)
C13—N3—C12—C11	103.6 (3)	O2—C31—C32—N7	−160.5 (2)
C20—N3—C12—C11	−76.4 (3)	O2—C31—C32A—N7A	175.8 (6)
O1—C11—C12—N3	−60.0 (3)	C31—C32—N7—C40	80.5 (3)
C15—N4—C13—N3	0.8 (3)	C31—C32—N7—C33	−106.9 (3)
C15—N4—C13—S2	−179.9 (2)	C35—N8—C33—N7	0.9
C20—N3—C13—N4	−0.6 (3)	C35—N8—C33—S4	−178.6
C12—N3—C13—N4	179.4 (2)	C40—N7—C33—N8	−1.4

C20—N3—C13—S2	−179.87 (19)	C32—N7—C33—N8	−175.1 (3)
C12—N3—C13—S2	0.1 (4)	C40—N7—C33—S4	178.2
C14—S2—C13—N4	−23.2 (3)	C32—N7—C33—S4	4.5 (3)
C14—S2—C13—N3	156.0 (3)	C34—S4—C33—N8	−1.8
C13—N4—C15—C16	178.5 (3)	C34—S4—C33—N7	178.7
C13—N4—C15—C20	−0.8 (3)	C33—N8—C35—C36	177.9
N4—C15—C16—C17	−178.7 (3)	C33—N8—C35—C40	−0.1
C20—C15—C16—C17	0.5 (4)	N8—C35—C36—C37	−177.3
C15—C16—C17—C18	−1.6 (5)	C40—C35—C36—C37	0.4
C16—C17—C18—C19	1.4 (6)	C35—C36—C37—C38	0.3
C17—C18—C19—C20	−0.1 (5)	C36—C37—C38—C39	−1.0
C18—C19—C20—N3	178.7 (3)	C37—C38—C39—C40	0.9
C18—C19—C20—C15	−1.0 (4)	C33—N7—C40—C39	−176.9
C13—N3—C20—C19	−179.6 (3)	C32—N7—C40—C39	−2.8 (3)
C12—N3—C20—C19	0.4 (4)	C33—N7—C40—C35	1.1
C13—N3—C20—C15	0.0 (3)	C32—N7—C40—C35	175.2 (3)
C12—N3—C20—C15	−180.0 (2)	C38—C39—C40—N7	177.7
C16—C15—C20—C19	0.8 (4)	C38—C39—C40—C35	−0.1
N4—C15—C20—C19	−179.8 (2)	C36—C35—C40—N7	−178.8
C16—C15—C20—N3	−178.9 (2)	N8—C35—C40—N7	−0.7
N4—C15—C20—N3	0.4 (3)	C36—C35—C40—C39	−0.6
C27—N6—C21—C22	−176.9	N8—C35—C40—C39	177.6
C29—N6—C21—C22	2.2 (2)	C31—C32A—N7A—C40A	−75.9 (9)
C27—N6—C21—C26	1.1	C31—C32A—N7A—C33A	94.9 (7)
C29—N6—C21—C26	−179.8 (2)	C35A—N8A—C33A—N7A	0.9
N6—C21—C22—C23	178.1	C35A—N8A—C33A—S4A	−178.6
C26—C21—C22—C23	0.3	C40A—N7A—C33A—N8A	−1.4
C21—C22—C23—C24	0.2	C32A—N7A—C33A—N8A	−173.6 (8)
C22—C23—C24—C25	−0.3	C40A—N7A—C33A—S4A	178.2
C23—C24—C25—C26	−0.2	C32A—N7A—C33A—S4A	6.0 (8)
C24—C25—C26—N5	−177.3	C34A—S4A—C33A—N8A	−1.8
C24—C25—C26—C21	0.7	C34A—S4A—C33A—N7A	178.7
C27—N5—C26—C25	178.0	C33A—N8A—C35A—C36A	177.9
C27—N5—C26—C21	−0.1	C33A—N8A—C35A—C40A	−0.1
N6—C21—C26—C25	−179.0	N8A—C35A—C36A—C37A	−177.3
C22—C21—C26—C25	−0.8	C40A—C35A—C36A—C37A	0.4
N6—C21—C26—N5	−0.7	C35A—C36A—C37A—C38A	0.3
C22—C21—C26—N5	177.6	C36A—C37A—C38A—C39A	−1.0
C26—N5—C27—N6	0.9	C37A—C38A—C39A—C40A	0.9
C26—N5—C27—S3	−178.4	C33A—N7A—C40A—C39A	−176.9
C21—N6—C27—N5	−1.3	C32A—N7A—C40A—C39A	−4.4 (8)
C29—N6—C27—N5	179.6 (2)	C33A—N7A—C40A—C35A	1.1
C21—N6—C27—S3	178.0	C32A—N7A—C40A—C35A	173.6 (8)
C29—N6—C27—S3	−1.0 (2)	C38A—C39A—C40A—N7A	177.7
C28—S3—C27—N5	−23.16 (19)	C38A—C39A—C40A—C35A	−0.1
C28—S3—C27—N6	157.56 (19)	C36A—C35A—C40A—N7A	−178.8
C29—N6A—C21A—C22A	15.0 (9)	N8A—C35A—C40A—N7A	−0.7
C27A—N6A—C21A—C22A	−176.9	C36A—C35A—C40A—C39A	−0.6

C29—N6A—C21A—C26A	−166.9 (9)	N8A—C35A—C40A—C39A	177.6
C27A—N6A—C21A—C26A	1.1		

Hydrogen-bond geometry (Å, º)

*Cg*1, *Cg*5 and *Cg*11 are the centroids of the N5/C26/C21/N6/C27, the C21-C26 and the C1–C6 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···*Cg*5^{i}	0.95	2.71	3.583 (3)	153
C11—H11*B*···*Cg*11^{ii}	0.99	2.74	3.423 (3)	126
C29—H29*B*···*Cg*1^{iii}	0.99	2.70	3.489 (3)	137
C34—H34*B*···N4^{iv}	0.98	2.50	3.398 (3)	153

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