Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

X-ray structural insights and computational analysis of the compound 5-ethyl-4-[(4-morpholinobenzylidene)amino]-2,4-dihydro-3*H*-1,2,4-triazole-3-thione

Syed Nizamuddin,[a,b] T. N. Mahadeva Prasad,[c] N. R. Sreenatha,[d]* C. L. Sharath,[e] B. N. Lakshminarayana[f] and K. A. Vishnumurthy[g]*

[a]Department of PG Studies and Research in Industrial Chemistry, Kuvempu University, Shivamogga, Karnataka, India, [b]Department of Chemistry, Adichunchanagiri Institute of Technology, Chikkamagaluru 577102, Karnataka, India, [c]Department of Physics, Government First Grade College, Gundlupet 571111, Karnataka, India, [d]Department of Physics, Government Engineering College, Chamarajanagara 571313, Karnataka, India, [e]Department of Studies in Chemistry, Mangalore University, Mangalagangothri, Mangaluru 574199, Karnataka, India, [f]Department of Physics, Adichunchanagiri Institute of Technology, Chikkamagaluru 577102, Karnataka, India, and [g]Retired Joint Director, Department of Collegiate Education, Government of Karnataka, Regional Office, Shivamogga, India. *Correspondence e-mail: srinath25683@gmail.com, drvishnumurthyka@gmail.com

Received 7 March 2025
Accepted 28 May 2025

Edited by F. Di Salvo, University of Buenos Aires, Argentina

Keywords: single crystal XRD; chair conformation; Hirshfeld surfaces; 2D fingerprint plots.

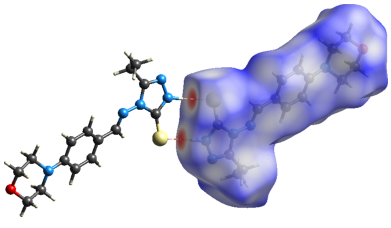
CCDC reference: 2312837

Supporting information: this article has supporting information at journals.iucr.org/e

The title compound, $C_{15}H_{19}N_5OS$, crystallizes in the monoclinic crystal system, space group $P2_1/c$. The molecule adopts a non-planar geometry. A significant feature of the structure is the puckered six-membered morpholine ring, which adopts a chair conformation. In the crystal, molecules are linked through intermolecular N—H···S hydrogen bonds, forming inversion-related dimers with an $R_2^2(8)$ ring motif. A Hirshfeld surface analysis was undertaken to quantify the intermolecular interactions that influence the crystal packing.

1. Chemical context

Heterocyclic compounds play a vital role in pharmaceutical research due to their wide range of biological activities. The present compound contains both a six-membered morpholine ring and a five-membered triazole moiety, each known for their therapeutic potential. Morpholine derivatives are also valued in industrial applications, such as corrosion inhibition in shale gas pipelines, owing to their low toxicity and antimicrobial properties (Wang *et al.*, 2024; Zhao *et al.*, 2024). Beyond pharmaceuticals, morpholine has gained attention for its use in fruit wax coatings, where its potential conversion to carcinogenic *N*-nitrosomorpholine highlights significant health risks and regulatory importance (Sundarrajan *et al.*, 2025). Additionally, *N*-heteroarylmorpholine frameworks are frequently found in drugs used to treat conditions such as schizophrenia and type-2 diabetes mellitus (Bandaru *et al.*, 2018).



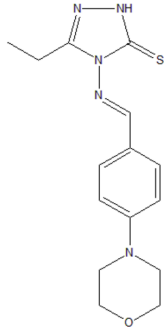


Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4N···S1^{i}	0.87 (4)	2.474 (4)	3.335 (2)	179 (14)

Symmetry code: (i) $-x, -y+1, -z$.

In the light of these diverse applications and biological significance, we report the structural and computational analysis of the compound 5-ethyl-4-[(4-morpholinobenzylidene)amino]-2,4-dihydro-3H-1,2,4-triazole-3-thione.

2. Structural commentary

The molecular structure is illustrated in Fig. 1. The molecule exhibits a slightly non-planar geometry. The dihedral angle between the mean planes of the morpholine ring (C1–C2–N1–C3–C4–O1) and the triazole ring (N3–C12–N4–N5–C13) is 11.42 (2)°, indicating a twisted conformation across the central phenyl ring (C5–C10). The morpholine ring adopts a chair conformation with puckering amplitude Q = 0.545 (3)Å, θ = 175.1 (3)° and relative phase angle of 177 (4)°. The ethyl side chain at C13 adopts a +syn-clinal orientation, as indicated by a N5—C13—C14—C15 torsion angle of 88.9 (5)°. The sulfur atom at C12 is in a +anti-periplanar arrangement with respect to the triazole ring, with a torsion angle of 176.5 (2)° for the chain of N5—N4—C12—S1 atoms. Bond lengths and angles are in good agreement with those in reported structures (Lakshminarayana *et al.*, 2022; Di Salvo *et al.*, 2011; Sreenatha *et al.*, 2017).

3. Supramolecular features

In the crystal, molecules are connected by intermolecular N4—H4N···S1 hydrogen bonds (Table 1), forming inversion dimers characterized by an $R_2^2(8)$ motif. The two-dimensional projection along the crystallographic b-axis direction is shown in Fig. 2. The packing mode along the crystallographic a-axis is shown in Fig. 3.

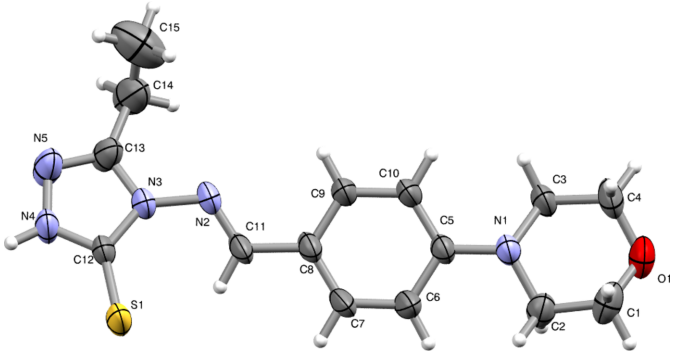


Figure 1
The molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level.

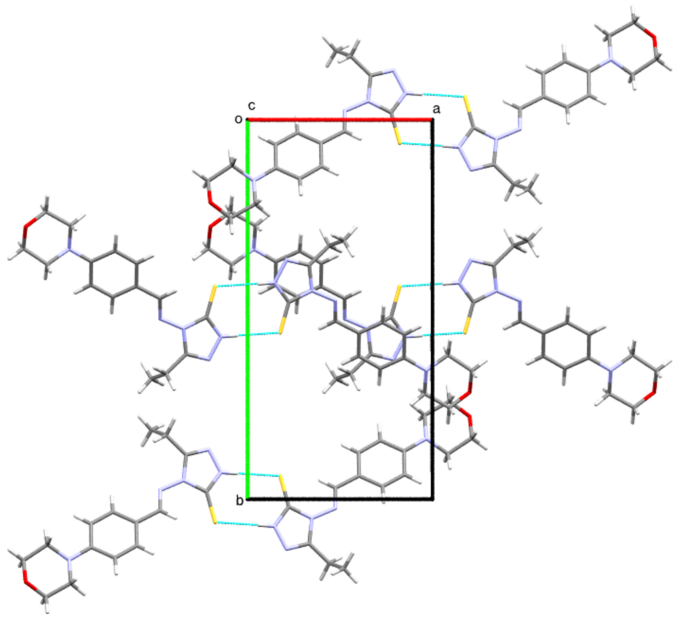


Figure 2
The packing of title molecules *via* intermolecular N4—H4N···S1 interactions, viewed along the crystallographic b-axis direction.

4. Database survey

A search of the Cambridge Structural Database (CSD,2025version; Groom *et al.*, 2016) for morpholine-containing compounds yielded numerous hits. Among them, AHEPUY (Oswald *et al.*, 2002) shows paracetamol molecules hydrogen-bonded *via* N—H···O and C═O···H interactions mediated by morpholine. The morpholine derivative AGAZAL (Sarbu *et al.*, 2013) exhibits O—H···O, C—H···O, and C—H···S interactions, supporting the relevance of such motifs in structural studies.

5. Hirshfeld surfaces and 2D fingerprint calculations

Hirshfeld surface analysis and corresponding fingerprint plots were generated using *CrystalExplorer* software. (Spackman *et*

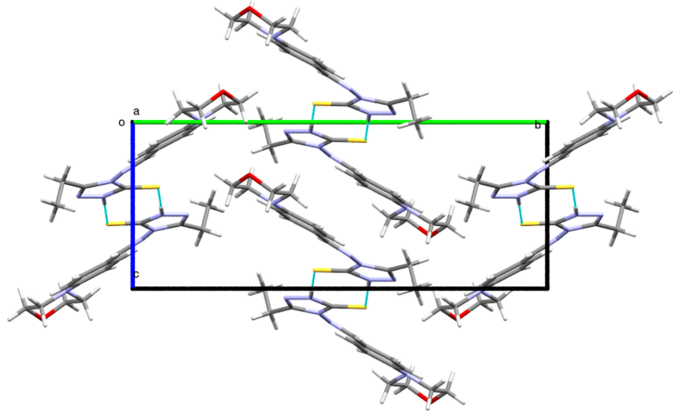


Figure 3
The packing viewed along the crystallographic a-axis direction.

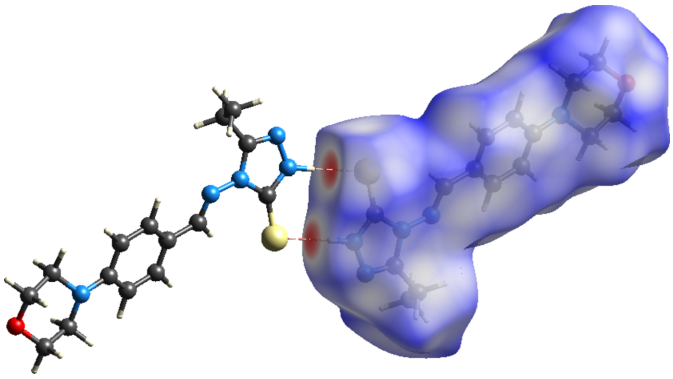


Figure 4
The Hirshfeld surface of the title compound mapped over d_{norm} with red spots corresponding to the intermolecular N4—H4*N*···S1 interactions.

al., 2021; Spackman & Jayatilaka, 2009). The surface mapped over d_{norm} shows red spots corresponding to regions of strong intermolecular interactions (Fig. 4). The 2D fingerprint plots (Fig. 5) quantify the contributions of various contact types: H···H interactions contribute the most at 52.6%, forming characteristic blue 'wings' around 1.01 Å. The S···H/H···S interactions contribute 13.4%, forming a distinct 'scorpion-pin' motif near $d_e + d_i \simeq 2.37$ Å. C···H/H···C contacts account for 10.4%, forming lung-shaped patterns at $d_e + d_i \simeq$ 2.91 Å. N···H/H···N contacts contribute 9.2%, appearing as spike-like features near $d_e + d_i \simeq 2.61$Å. O···H/H···O contacts contribute 5.9%, forming wing-like shapes at $d_e + d_i \simeq 2.71$Å

6. Synthesis and crystallization

An equimolar mixture of *p*-morpholinobenzaldehyde (**1**) and 4-amino-5-ethyl-4*H*-1,2,4-triazole-3-thiol (**2**) was refluxed in ethanol (10 mL) with a few drops of acetic acid for 6 h. Reaction progress was monitored by TLC. After completion,

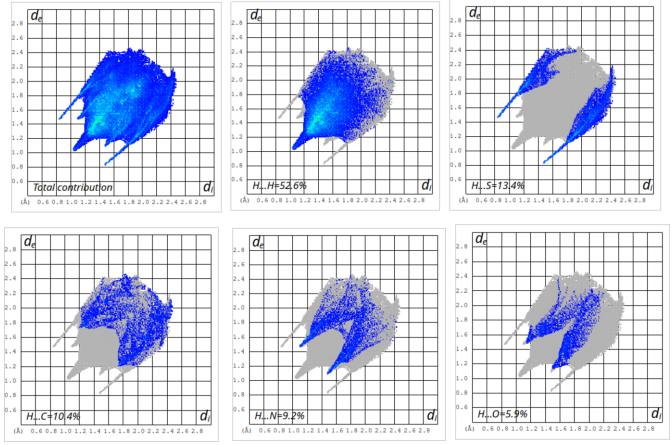


Figure 5
Two-dimensional fingerprint graphs showing the total contribution and those delineated into H···H, S···H/H···S, C···H/H···C, N···H/H···N and O···H/H···O contacts.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_{19}N_5OS$
M_r	317.41
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	9.7280 (8), 19.9593 (15), 8.0087 (6)
β (°)	93.230 (4)
V (Å^3)	1552.5 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.22
Crystal size (mm)	0.80 × 0.70 × 0.60
Data collection	
Diffractometer	Bruker SMART APEX
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	16741, 3824, 2528
R_{int}	0.043
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.670
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.063, 0.193, 1.01
No. of reflections	3824
No. of parameters	204
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.71, −0.55

Computer programs: *APEX* and *SAINT* (Bruker, 2006), *SHELXT2014/4* (Sheldrick, 2015*a*), *SHELXL2019/2* (Sheldrick, 2015*b*) and *PLATON*(Spek, 2020).

the solution was cooled to room temperature. The resulting solid was filtered, dried, and recrystallized from ethanol solution to obtain crystals suitable for X-ray analysis. A reaction scheme is provided in Fig. 6 (for more details of the synthesis, see:Dhaka *et al.*, 1974; Liu & Yan, 2008). The crystallized compound corresponds to the thione form (**3b**), which may be favored in the solid state due to possible intermolecular N4—H4*N*···S1 hydrogen-bonding interactions in the crystal. However, similar stabilizing forces could also operate in the thiol tautomer (**3a**).

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. C-bound hydrogen atoms were placed in idealized positions and refined as riding with C—H =

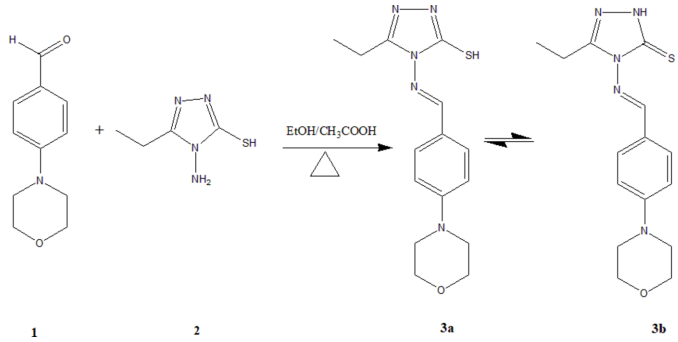


Figure 6
The synthesis scheme for the title compound.

0.93 Å with U_{iso}(H) = 1.2U_{eq}(C). The NH atom was freely refined.

Acknowledgements

The authors are are grateful to the Department of Physics, Adichunchanagiri Institute of Technology, Chikkamagaluru, and Government Engineering College, Chamarajanagara 571313, Karnataka, India for support and also thank the SAIF, IIT Madras, Chennai-36,Tamil Nadu, India, for the XRD data collection.

References

Bandaru, S. S. M., Kapdi, A. R. & Schulzke, C. (2018). *Acta Cryst.* E**74**, 137–140.

Bruker (2006). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.

Dhaka, K. S., Jag Mohan, Chanda, V. K., Pujari, H. K., (1974). *Indian J. Chem.* **12** 288.

Di Salvo, F., Camargo, B., García, Y., Teixidor, F., Viñas, C., Planas, J., Light, M. E. & Hursthouse, M. B. (2011). *CrystEngComm* **13**, 5788–5806.

Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.

Lakshminarayana, B. N., Sreenatha, N. R., Jeevan Chakravarthy, A. S., Suchithra, B. & Hariprasad, S. (2022). *Crystallogr. Rep.* **67**, 201–208.

Liu, J. L. & Yan, B. (2008). *J. Phys. Chem. C*, **112**, 14168–14178.

Oswald, I. D. H., Motherwell, W. D. S., Parsons, S. & Pulham, C. R. (2002). *Acta Cryst.* E**58**, o1290–o1292.

Sarbu, L. G., Hrib, C. G. & Birsa, L. M. (2013). *Acta Cryst.* E**69**, o1169.

Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.

Sheldrick, G. M. (2015*b*). *Acta Cryst.* A**71**, 3–8.

Spackman, M. A. & Jayatilaka, D. (2009). *CrystEngComm* **11**, 19–32.

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.

Spek, A. L. (2020). *Acta Cryst.* E**76**, 1–11.

Sreenatha, N. R., Lakshminarayana, B. N., Mahadeva Prasad, T. N., Vijayshankar, S. & Byrappa, K. (2017). *Chem. Data Collect.* **11**, 131–138.

Sundarrajan, B., Paduvetnaya, L., Prabhu, A., Basavaraj, S., Harishkkumar, M. & Naresh kumar, M. (2025). *Food Anal. Methods* 1–12. https://doi.org/10.1007/s12161-025-02791-1

Wang, T., Dai, S., Xiong, Y., Yan, H. & Zhu, Y. (2024). *Colloids Surf. A: Physicochem. Eng. Asp.* **700**, 134784. https://doi.org/10.1016/j.colsurfa.2024.134784.

Zhao, X., Zhang, J., Ma, L., Wang, W. & Zhang, M. (2024). *Coatings* **14**, 997. https://doi.org/10.3390/coatings14080997

supporting information

Acta Cryst. (2025). E**81**, 565-568 [https://doi.org/10.1107/S2056989025004852]

X-ray structural insights and computational analysis of the compound 5-ethyl-4-[(4-morpholinobenzylidene)amino]-2,4-dihydro-3*H*-1,2,4-triazole-3-thione

Syed Nizamuddin, T. N. Mahadeva Prasad, N. R. Sreenatha, C. L. Sharath, B. N. Lakshminarayana and K. A. Vishnumurthy

Computing details

5-Ethyl-4-[(4-morpholinobenzylidene)amino]-2,4-dihydro-3*H*-1,2,4-triazole-3-thione

Crystal data

$C_{15}H_{19}N_5OS$
$M_r = 317.41$
Monoclinic, $P2_1/c$
$a = 9.7280$ (8) Å
$b = 19.9593$ (15) Å
$c = 8.0087$ (6) Å
$\beta = 93.230$ (4)°
$V = 1552.5$ (2) Å^3
$Z = 4$
$F(000) = 672$
$D_x = 1.358$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3824 reflections
$\theta = 2.3$–$28.4°$
$\mu = 0.22$ mm^{-1}
$T = 296$ K
Block, colorless
0.80 × 0.70 × 0.60 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: graphite
Detector resolution: 0.812 pixels mm^{-1}
16741 measured reflections
3824 independent reflections
2528 reflections with $I > 2\sigma(I)$
$R_{int} = 0.043$
$\theta_{max} = 28.4°$, $\theta_{min} = 2.3°$
$h = -12 \rightarrow 13$
$k = -26 \rightarrow 26$
$l = -10 \rightarrow 10$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.063$
$wR(F^2) = 0.193$
$S = 1.01$
3824 reflections
204 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.091P)^2 + 1.1496P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.71$ e Å^{-3}
$\Delta\rho_{min} = -0.55$ e Å^{-3}

Special details

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	1.0926 (3)	0.75825 (16)	0.6166 (4)	0.0617 (8)
H1A	1.113183	0.772682	0.505069	0.074*
H1B	1.084745	0.797943	0.685299	0.074*
C2	0.9581 (3)	0.72168 (13)	0.6080 (4)	0.0505 (7)
H2A	0.932333	0.711318	0.720376	0.061*
H2B	0.887212	0.750150	0.555856	0.061*
C3	1.0849 (2)	0.61946 (14)	0.5713 (4)	0.0517 (7)
H3A	1.095855	0.582320	0.495109	0.062*
H3B	1.068877	0.601234	0.680808	0.062*
C4	1.2142 (3)	0.66126 (18)	0.5813 (4)	0.0648 (9)
H4A	1.290469	0.634002	0.625262	0.078*
H4B	1.234677	0.675563	0.469684	0.078*
C5	0.8470 (2)	0.62665 (12)	0.4614 (3)	0.0388 (5)
C6	0.7183 (3)	0.65485 (17)	0.4808 (4)	0.0639 (9)
H6	0.711682	0.696074	0.533834	0.077*
C7	0.6005 (3)	0.62238 (18)	0.4223 (4)	0.0666 (10)
H7	0.515733	0.642494	0.436839	0.080*
C8	0.6032 (2)	0.56162 (14)	0.3435 (3)	0.0431 (6)
C9	0.7306 (2)	0.53358 (13)	0.3225 (4)	0.0452 (6)
H9	0.736421	0.492724	0.267475	0.054*
C10	0.8490 (2)	0.56506 (13)	0.3814 (4)	0.0497 (7)
H10	0.933271	0.544418	0.367359	0.060*
C11	0.4752 (2)	0.52978 (15)	0.2829 (3)	0.0490 (7)
H11	0.391832	0.549583	0.305837	0.059*
C12	0.2230 (2)	0.48038 (13)	0.1063 (3)	0.0410 (6)
C13	0.3334 (3)	0.38280 (15)	0.1116 (4)	0.0602 (8)
C14	0.4417 (4)	0.3313 (2)	0.1434 (5)	0.0869 (13)
H14A	0.503355	0.346216	0.235420	0.104*
H14B	0.398600	0.290136	0.177690	0.104*
C15	0.5207 (5)	0.3176 (3)	0.0030 (7)	0.1182 (18)
H15A	0.460516	0.303478	−0.089486	0.177*
H15B	0.585800	0.282663	0.031072	0.177*
H15C	0.568966	0.357333	−0.027256	0.177*
N1	0.9671 (2)	0.66008 (10)	0.5129 (3)	0.0427 (5)
N2	0.4746 (2)	0.47624 (12)	0.2003 (3)	0.0460 (5)
N3	0.3474 (2)	0.44995 (11)	0.1461 (3)	0.0439 (5)
N4	0.1450 (2)	0.42896 (11)	0.0544 (3)	0.0497 (6)
N5	0.2104 (3)	0.36884 (12)	0.0545 (4)	0.0646 (7)
O1	1.2022 (2)	0.71815 (11)	0.6838 (3)	0.0642 (6)

S1	0.17662 (7)	0.56092 (4)	0.11137 (12)	0.0624 (3)
H4N	0.061 (4)	0.4319 (17)	0.012 (4)	0.074 (11)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.073 (2)	0.0510 (16)	0.0588 (18)	−0.0207 (15)	−0.0122 (15)	−0.0001 (14)
C2	0.0502 (15)	0.0419 (14)	0.0578 (16)	−0.0028 (12)	−0.0111 (12)	−0.0004 (12)
C3	0.0281 (12)	0.0526 (15)	0.0730 (18)	0.0009 (11)	−0.0091 (12)	−0.0053 (14)
C4	0.0321 (13)	0.083 (2)	0.078 (2)	−0.0113 (14)	−0.0091 (13)	−0.0072 (17)
C5	0.0269 (11)	0.0447 (13)	0.0439 (13)	0.0000 (9)	−0.0042 (9)	0.0006 (10)
C6	0.0363 (14)	0.069 (2)	0.084 (2)	0.0110 (13)	−0.0127 (13)	−0.0383 (17)
C7	0.0249 (12)	0.090 (2)	0.084 (2)	0.0134 (13)	−0.0087 (13)	−0.0391 (19)
C8	0.0251 (11)	0.0588 (16)	0.0445 (13)	0.0011 (10)	−0.0052 (9)	−0.0064 (12)
C9	0.0295 (12)	0.0406 (13)	0.0647 (16)	0.0010 (10)	−0.0041 (11)	−0.0086 (12)
C10	0.0249 (11)	0.0463 (14)	0.0773 (19)	0.0018 (10)	−0.0011 (11)	−0.0094 (13)
C11	0.0215 (11)	0.0739 (19)	0.0510 (15)	0.0030 (11)	−0.0045 (10)	−0.0131 (14)
C12	0.0249 (10)	0.0449 (13)	0.0525 (14)	−0.0041 (9)	−0.0027 (10)	−0.0029 (11)
C13	0.0618 (18)	0.0494 (16)	0.0659 (18)	0.0105 (14)	−0.0268 (15)	−0.0133 (14)
C14	0.082 (3)	0.074 (2)	0.100 (3)	0.025 (2)	−0.042 (2)	−0.022 (2)
C15	0.088 (3)	0.133 (4)	0.135 (4)	0.035 (3)	0.021 (3)	0.032 (3)
N1	0.0295 (10)	0.0418 (11)	0.0558 (12)	−0.0025 (8)	−0.0054 (9)	−0.0015 (10)
N2	0.0245 (10)	0.0561 (13)	0.0564 (13)	−0.0006 (9)	−0.0080 (9)	−0.0049 (11)
N3	0.0294 (10)	0.0480 (12)	0.0529 (12)	0.0002 (9)	−0.0095 (9)	−0.0071 (10)
N4	0.0333 (11)	0.0439 (12)	0.0700 (15)	−0.0059 (9)	−0.0142 (10)	−0.0016 (11)
N5	0.0621 (16)	0.0446 (13)	0.0829 (18)	0.0005 (11)	−0.0334 (14)	−0.0060 (12)
O1	0.0509 (12)	0.0719 (14)	0.0674 (13)	−0.0175 (10)	−0.0176 (10)	−0.0056 (11)
S1	0.0338 (4)	0.0461 (4)	0.1046 (7)	0.0026 (3)	−0.0201 (4)	−0.0148 (4)

Geometric parameters (Å, º)

C1—O1	1.415 (4)	C8—C11	1.457 (3)
C1—C2	1.496 (4)	C9—C10	1.372 (3)
C1—H1A	0.9700	C9—H9	0.9300
C1—H1B	0.9700	C10—H10	0.9300
C2—N1	1.452 (3)	C11—N2	1.256 (3)
C2—H2A	0.9700	C11—H11	0.9300
C2—H2B	0.9700	C12—N4	1.329 (3)
C3—N1	1.459 (3)	C12—N3	1.375 (3)
C3—C4	1.508 (4)	C12—S1	1.671 (3)
C3—H3A	0.9700	C13—N5	1.287 (4)
C3—H3B	0.9700	C13—N3	1.374 (4)
C4—O1	1.409 (4)	C13—C14	1.483 (4)
C4—H4A	0.9700	C14—C15	1.424 (6)
C4—H4B	0.9700	C14—H14A	0.9700
C5—C10	1.387 (4)	C14—H14B	0.9700
C5—N1	1.388 (3)	C15—H15A	0.9600
C5—C6	1.390 (4)	C15—H15B	0.9600

C6—C7	1.376 (4)	C15—H15C	0.9600
C6—H6	0.9300	N2—N3	1.391 (3)
C7—C8	1.368 (4)	N4—N5	1.358 (3)
C7—H7	0.9300	N4—H4N	0.87 (4)
C8—C9	1.379 (3)		

O1—C1—C2	112.3 (2)	C8—C9—H9	119.5
O1—C1—H1A	109.1	C9—C10—C5	122.1 (2)
C2—C1—H1A	109.1	C9—C10—H10	118.9
O1—C1—H1B	109.1	C5—C10—H10	118.9
C2—C1—H1B	109.1	N2—C11—C8	121.7 (2)
H1A—C1—H1B	107.9	N2—C11—H11	119.2
N1—C2—C1	111.0 (2)	C8—C11—H11	119.2
N1—C2—H2A	109.4	N4—C12—N3	102.2 (2)
C1—C2—H2A	109.4	N4—C12—S1	126.90 (19)
N1—C2—H2B	109.4	N3—C12—S1	130.90 (19)
C1—C2—H2B	109.4	N5—C13—N3	111.3 (2)
H2A—C2—H2B	108.0	N5—C13—C14	123.3 (3)
N1—C3—C4	110.3 (2)	N3—C13—C14	125.4 (3)
N1—C3—H3A	109.6	C15—C14—C13	114.1 (4)
C4—C3—H3A	109.6	C15—C14—H14A	108.7
N1—C3—H3B	109.6	C13—C14—H14A	108.7
C4—C3—H3B	109.6	C15—C14—H14B	108.7
H3A—C3—H3B	108.1	C13—C14—H14B	108.7
O1—C4—C3	112.3 (3)	H14A—C14—H14B	107.6
O1—C4—H4A	109.1	C14—C15—H15A	109.5
C3—C4—H4A	109.1	C14—C15—H15B	109.5
O1—C4—H4B	109.1	H15A—C15—H15B	109.5
C3—C4—H4B	109.1	C14—C15—H15C	109.5
H4A—C4—H4B	107.9	H15A—C15—H15C	109.5
C10—C5—N1	122.0 (2)	H15B—C15—H15C	109.5
C10—C5—C6	116.5 (2)	C5—N1—C2	119.3 (2)
N1—C5—C6	121.4 (2)	C5—N1—C3	117.4 (2)
C7—C6—C5	120.7 (3)	C2—N1—C3	111.8 (2)
C7—C6—H6	119.7	C11—N2—N3	117.6 (2)
C5—C6—H6	119.7	C13—N3—C12	107.9 (2)
C8—C7—C6	122.5 (2)	C13—N3—N2	120.5 (2)
C8—C7—H7	118.8	C12—N3—N2	131.4 (2)
C6—C7—H7	118.8	C12—N4—N5	115.0 (2)
C7—C8—C9	117.2 (2)	C12—N4—H4N	125 (2)
C7—C8—C11	120.1 (2)	N5—N4—H4N	119 (2)
C9—C8—C11	122.7 (2)	C13—N5—N4	103.6 (2)
C10—C9—C8	121.0 (2)	C4—O1—C1	108.7 (2)
C10—C9—H9	119.5		

O1—C1—C2—N1	−56.1 (3)	C1—C2—N1—C3	51.0 (3)
N1—C3—C4—O1	56.2 (3)	C4—C3—N1—C5	166.0 (2)
C10—C5—C6—C7	−0.1 (5)	C4—C3—N1—C2	−50.7 (3)

N1—C5—C6—C7	177.1 (3)	C8—C11—N2—N3	−179.3 (2)
C5—C6—C7—C8	0.1 (6)	N5—C13—N3—C12	−0.4 (4)
C6—C7—C8—C9	−0.7 (5)	C14—C13—N3—C12	−177.2 (3)
C6—C7—C8—C11	−179.5 (3)	N5—C13—N3—N2	−176.4 (3)
C7—C8—C9—C10	1.2 (4)	C14—C13—N3—N2	6.8 (5)
C11—C8—C9—C10	−180.0 (3)	N4—C12—N3—C13	1.0 (3)
C8—C9—C10—C5	−1.3 (5)	S1—C12—N3—C13	−176.7 (2)
N1—C5—C10—C9	−176.5 (3)	N4—C12—N3—N2	176.4 (3)
C6—C5—C10—C9	0.7 (4)	S1—C12—N3—N2	−1.3 (4)
C7—C8—C11—N2	175.2 (3)	C11—N2—N3—C13	−156.1 (3)
C9—C8—C11—N2	−3.6 (5)	C11—N2—N3—C12	29.0 (4)
N5—C13—C14—C15	88.9 (5)	N3—C12—N4—N5	−1.4 (3)
N3—C13—C14—C15	−94.5 (5)	S1—C12—N4—N5	176.5 (2)
C10—C5—N1—C2	−175.0 (2)	N3—C13—N5—N4	−0.5 (4)
C6—C5—N1—C2	8.0 (4)	C14—C13—N5—N4	176.5 (3)
C10—C5—N1—C3	−34.5 (4)	C12—N4—N5—C13	1.2 (4)
C6—C5—N1—C3	148.4 (3)	C3—C4—O1—C1	−60.1 (3)
C1—C2—N1—C5	−166.5 (2)	C2—C1—O1—C4	59.9 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4*N*···S1^{i}	0.87 (4)	2.474 (4)	3.335 (2)	179 (14)

Symmetry code: (i) −*x*, −*y*+1, −*z*.