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Crystal structure of (2*Z*,5*Z*)-3-(4-methoxyphenyl)-2-[(4-methoxyphenyl)imino]-5-[(*E*)-3-(2-nitrophenyl)-allylidene]-1,3-thiazolidin-4-one

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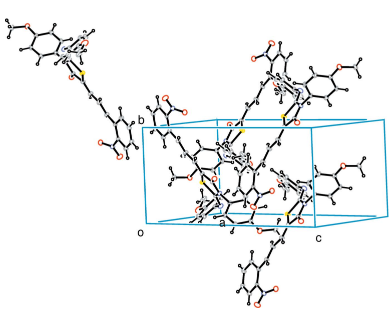
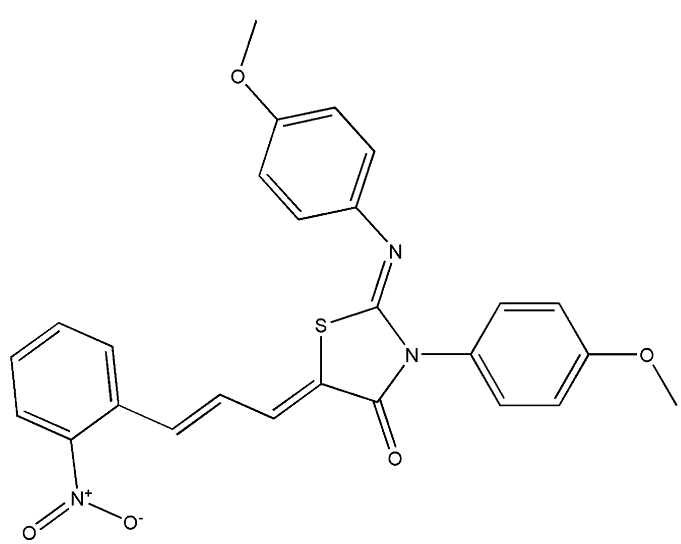
In the title compound, $C_{26}H_{21}N_3O_5S$, the thiazole ring is nearly planar with a maximum deviation of 0.017 (2) Å, and is twisted with respect to the three benzene rings, making dihedral angles of 25.52 (12), 85.77 (12) and 81.85 (13)°. In the crystal, weak C—H⋯O hydrogen bonds and C—H⋯π interactions link the molecules into a three-dimensional supramolecular architecture. Aromatic π–π stacking is also observed between the parallel nitrobenzene rings of neighbouring molecules, the centroid-to-centroid distance being 3.5872 (15) Å.

1. Chemical context

Heterocycles containing a thiazole ring are found to exhibit a wide spectrum of biological activities (Gautam *et al.*, 2015; Asif, 2015; Abhinit *et al.*, 2009). The thiazolidinones that are used widely in medication are derived from thiazolidines containing sulfur and nitrogen in a five-membered ring (Meera *et al.*, 2014; Nowaczyk *et al.*, 2014; Toubal *et al.*, 2012). Knowledge of the crystal structures of these compounds is crucial for understanding the related biological phenomena (Singh *et al.*, 1981; Ameta *et al.*, 2014; Gouda *et al.*, 2011). As part of our studies in this area, we herein report the synthesis and crystal structure of the title compound.





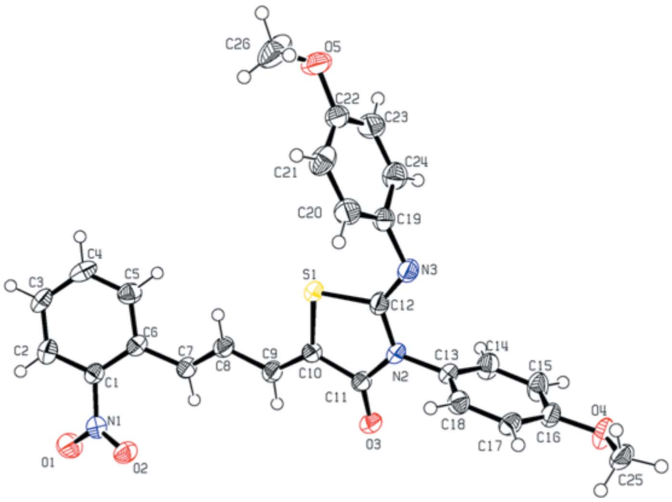


Figure 1
The molecular structure of the title compound showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

2. Structural commentary

The molecular structure with atomic numbering scheme for the title compound is given in Fig. 1. The N2—C11 and N2—C12 bond lengths [1.385 (3) and 1.389 (3) Å] are intermediate between the classical C—N single-bond length (1.47 Å) and C═N double-bond length (1.27 Å) (Bhagavan, 2002), indicating that the thiazole moiety is an effective electron-conjugated substructure. The C—S bond lengths in the thiazol rings [S1—C10 = 1.753 (3) and S1—C12 = 1.777 (2) Å] are consistant with the normal Csp^2—S single bond length of 1.76 Å (Sarkar *et al.*, 1984). The C16—O4 bond length [1.365 (3) Å] and C22—O5 bond length [1.375 (3) Å] are notably shorter than the normal O—C single bond (1.427 Å) (Rong Wan *et al.*, 2008), indicating that the *p* orbital occupied lone pair electrons of the oxygen atom in CH_3O and the π orbital in the benzene ring has *p*–π conjugation. The shorter bond length of C26—O5 [1.385 (5) Å] might be also caused by the delocalized electron density of the conjugated benzene ring. The C25—O4 [1.431 (3) Å] bond length is normal for a C—O single bond.

The thiazole ring is nearly planar with a maximum deviation of 0.017 (2) Å, and is twisted with respect to the three benzene rings, making dihedral angles of 25.52 (12), 85.77 (12) and 81.85 (13)°with the C1–C6, C13–C18 and C19–C24 rings, respectively.

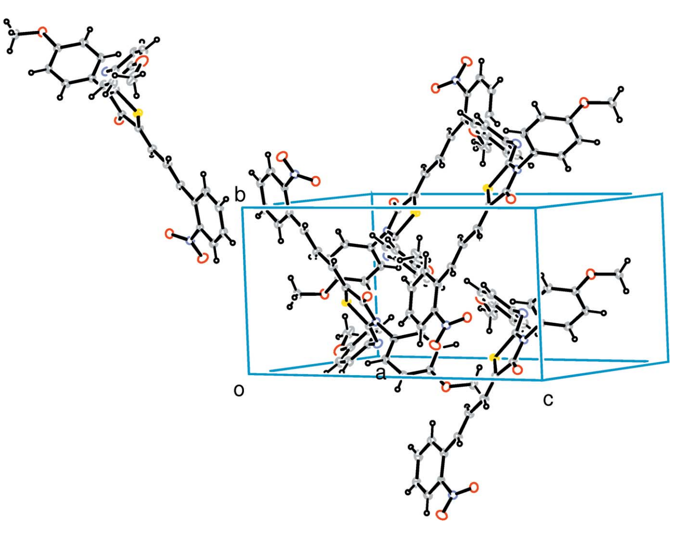


Figure 2
The crystal packing diagram showing π–π stacking between the nitrobenzene rings of the neighbouring molecules.

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

*Cg*3 is the centroid of the C13–C18 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···O3^{i}	1.00 (2)	2.55 (2)	3.197 (3)	122 (1)
C9—H9···O2^{ii}	0.97 (2)	2.58 (2)	3.400 (3)	142 (1)
C15—H15···O1^{iii}	0.93	2.59	3.286 (3)	132
C3—H3···*Cg*3^{iv}	0.93	2.80	3.560 (3)	140

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

3. Supramolecular features

In the crystal, weak C—H···O hydrogen bonds and C—H···π interactions (Table 1, Fig. 2) link the molecules into a three-dimensional supramolecular architecture. π–π stacking is also observed between the nearly parallel benzene rings of neighbouring molecules, the centroid-to-centroid distance being 3.5872 (15) Å.

4. Synthesis and crystallization

The synthesis of the title compound was performed according to the scheme in Fig. 3. To a solution of **3** (0.01 mol) in 10 mL of acetic acid and three equivalents of anhydrous sodium acetate was added 2-nitrophenylcinamaldehyde (0.01 mol). The mixture was heated at reflux with stirring, using CH_2Cl_2 (20 mL) for 4 h. The reaction was monitored by TLC using $CH_2Cl_2/CH_3CO_2C_2H_5$ (9/1) as solvent system. The separated solid was filtered, washed with cold water and dried to give a yellow solid with a moderate yield 75% and melting point 484 K. Single crystals of the title compound suitable for X-ray diffraction were obtained from an ethanol solution.

IR (KBr, cm^{-1}): 3423.03, 2951 (C—H), 1712 (C═O), 1640.16 (C═N), 1509.93 (C═C), 1030 (C—N), 741(C—S). ^{1}H NMR, ($CDCl_3$, 300 MHz) δ (p.p.m.) *J* (Hz): 3.81 (*s*, 3H, OCH_3), 3.85 (*s*, 3H, OCH_3), 6.71 (*dd*, 1H, *J* = 15.0 Hz, *J* = 11.55 Hz, CH), 6.90 (*s*, 4H, Ar-H), 7.04 (*d*, 2H, *J* = 8.8 Hz, Ar-H), 7.35 (*d*, 2H, *J* = 8.8 Hz, Ar-H), 7.43–7.67 (*m*, 5H, Ar-H), 8.0 (*d*, 1H, *J* = 8.72 Hz, Chet═CH). ^{13}C NMR, ($CDCl_3$, 300 MHz) δ (p.p.m.): 55.57 (O—CH_3), 55.65 (O—CH_3), 114.57, 114.85, 122.34, 125.22, 126.37, 127.35, 127.99, 128.50, 129.20, 129.57, 129.60, 131.61, 133.36, 135.79, 141.83, 148.13, 150.72, 157.20 (Chet═C), 159.90 (C═N), 165.87 (C═O).

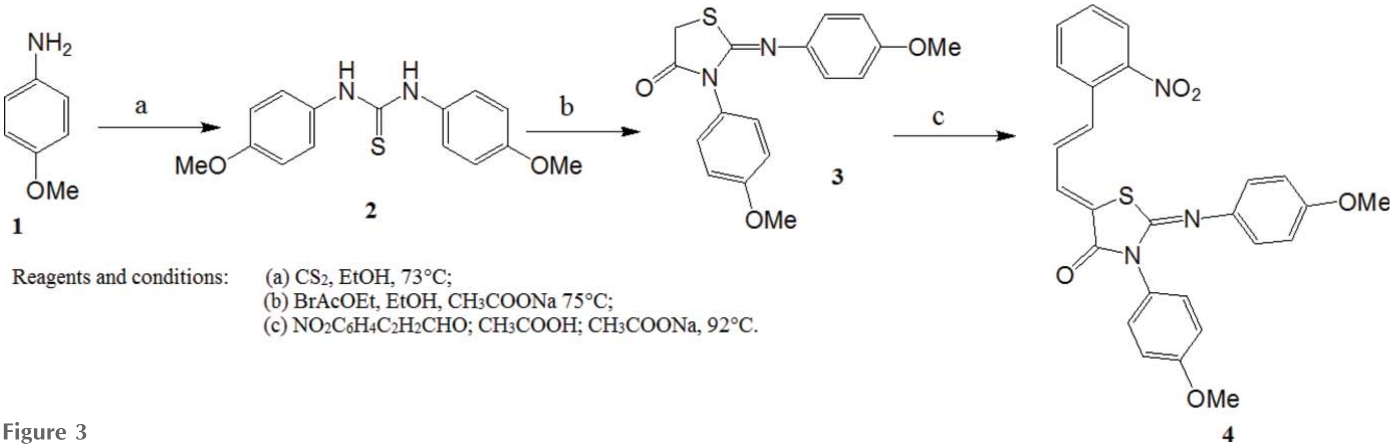


Figure 3
Chemical pathway showing the formation of the title compound.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms in the title compound were placed in calculated positions (C—H = 0.96–1.08 Å) and allowed to ride on their parent atoms with $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H atoms and $1.2U_{eq}(C)$ for other H atoms.

Acknowledgements

We gratefully acknowledge financial support from the Ministère de l'Enseignement Supérieur et de la Recherche Scientifique (MESRS) *via* the CNEPRU project.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{26}H_{21}N_3O_5S$
M_r	487.52
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	173
a, *b*, *c* (Å)	13.2727 (10), 8.6401 (4), 21.3018 (12)
β (°)	105.316 (7)
V (Å^3)	2356.1 (3)
Z	4
Radiation type	Mo *Kα*
μ (mm^{-1})	0.18
Crystal size (mm)	0.25 × 0.21 × 0.12
Data collection	
Diffractometer	Nonius Kappa CCD
Absorption correction	ψ scan (North *et al.*, 1968)
T_{min}, T_{max}	0.856, 0.919
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	26882, 5954, 3690
R_{int}	0.062
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.692
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.064, 0.166, 1.02
No. of reflections	5954
No. of parameters	322
H-atom treatment	H-atom parameters not refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.49, −0.34

Computer programs: *KappaCCD* (Nonius, 1998), *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997), *SHELXS97* (Sheldrick, 2008), *SHELXL2014*/7 (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012), and *Mercury* (Macrae *et al.*, 2006).

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Crystal structure of (2*Z*,5*Z*)-3-(4-methoxyphenyl)-2-[(4-methoxyphenyl)-imino]-5-[(*E*)-3-(2-nitrophenyl)allylidene]-1,3-thiazolidin-4-one

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Computing details

Data collection: Kappa CCD (Nonius, 1998); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014*/7 (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXL2014* (Sheldrick, 2015).

(2*Z*,5*Z*)-3-(4-Methoxyphenyl)-2-[(4-methoxyphenyl)imino]-5-[(*E*)-3-(2-nitrophenyl)allylidene]-1,3-thiazolidin-4-one

Crystal data

$C_{26}H_{21}N_3O_5S$
M_r = 487.52
Monoclinic, $P2_1/c$
a = 13.2727 (10) Å
b = 8.6401 (4) Å
c = 21.3018 (12) Å
β = 105.316 (7)°
V = 2356.1 (3) Å^3
Z = 4
F(000) = 1016
D_x = 1.374 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 100 reflections
θ = 2–29°
μ = 0.18 mm^{-1}
T = 173 K
Prism, yellow
0.25 × 0.21 × 0.12 mm

Data collection

Nonius Kappa CCD diffractometer
$\theta/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.856, T_{max} = 0.919
26882 measured reflections
5954 independent reflections
3690 reflections with $I > 2\sigma(I)$
R_{int} = 0.062
θ_{max} = 29.5°, θ_{min} = 2.9°
$h = -17 \rightarrow 17$
$k = -11 \rightarrow 11$
$l = -29 \rightarrow 27$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.166
S = 1.02
5954 reflections
322 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters not refined

$w = 1/[\sigma^2(F_o^2) + (0.0731P)^2 + 0.7139P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.49$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}

Special details

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

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

	x	y	z	U_{iso}*/U_{eq}
S1	0.28022 (6)	0.41002 (7)	0.22265 (3)	0.0317 (2)
O3	0.14135 (16)	0.4595 (2)	0.35874 (8)	0.0356 (5)
O4	0.29886 (17)	−0.0889 (2)	0.54702 (9)	0.0448 (5)
O2	0.08864 (16)	1.1504 (2)	0.22010 (8)	0.0389 (5)
N2	0.25988 (18)	0.2956 (2)	0.33219 (9)	0.0294 (5)
O1	−0.00470 (18)	1.3059 (2)	0.14901 (10)	0.0498 (6)
N3	0.37138 (19)	0.1521 (2)	0.28522 (10)	0.0345 (5)
N1	0.05420 (18)	1.1947 (2)	0.16354 (11)	0.0335 (5)
C11	0.1930 (2)	0.4215 (3)	0.32243 (12)	0.0287 (6)
C18	0.3513 (2)	0.2234 (3)	0.44293 (12)	0.0320 (6)
H18	0.3978	0.3040	0.4433	0.038*
C13	0.2708 (2)	0.1963 (3)	0.38783 (11)	0.0283 (6)
C10	0.1968 (2)	0.5044 (3)	0.26177 (12)	0.0295 (6)
C1	0.0854 (2)	1.1147 (3)	0.11192 (11)	0.0277 (6)
C8	0.1515 (2)	0.7251 (3)	0.18670 (12)	0.0326 (6)
H8	0.1950 (14)	0.6898 (12)	0.1613 (8)	0.039*
C19	0.4160 (2)	0.1407 (3)	0.23137 (12)	0.0335 (6)
C17	0.3631 (2)	0.1318 (3)	0.49738 (12)	0.0295 (6)
H17	0.4172	0.1505	0.5344	0.035*
C6	0.1071 (2)	0.9552 (3)	0.11536 (11)	0.0290 (6)
C9	0.1448 (2)	0.6358 (3)	0.24244 (12)	0.0324 (6)
H9	0.0994 (15)	0.6736 (12)	0.2677 (8)	0.039*
O5	0.5431 (2)	0.0888 (3)	0.07390 (10)	0.0618 (7)
C7	0.0979 (2)	0.8569 (3)	0.16964 (12)	0.0304 (6)
H7	0.0486 (15)	0.8903 (10)	0.1956 (8)	0.037*
C12	0.3111 (2)	0.2662 (3)	0.28442 (11)	0.0300 (6)
C16	0.2929 (2)	0.0105 (3)	0.49635 (12)	0.0325 (6)
C2	0.0961 (2)	1.2058 (3)	0.06006 (12)	0.0370 (7)
H2	0.0823	1.3114	0.0597	0.044*
C14	0.2003 (2)	0.0780 (3)	0.38674 (13)	0.0396 (7)
H14	0.1461	0.0606	0.3496	0.047*
C5	0.1365 (2)	0.8925 (3)	0.06228 (12)	0.0363 (6)
H5	0.1494	0.7867	0.0618	0.044*
C3	0.1275 (2)	1.1394 (3)	0.00918 (12)	0.0368 (7)
H3	0.1354	1.1995	−0.0254	0.044*
C4	0.1471 (2)	0.9813 (4)	0.01070 (13)	0.0412 (7)

H4	0.1675	0.9350	−0.0234	0.049*
C25	0.3914 (2)	−0.0808 (3)	0.59982 (12)	0.0404 (7)
H25A	0.4516	−0.0953	0.5835	0.061*
H25B	0.3894	−0.1603	0.6310	0.061*
H25C	0.3952	0.0187	0.6204	0.061*
C24	0.3733 (2)	0.0413 (3)	0.18017 (14)	0.0422 (7)
H24	0.3152	−0.0181	0.1807	0.051*
C21	0.5481 (2)	0.2158 (4)	0.17753 (14)	0.0438 (7)
H21	0.6056	0.2763	0.1764	0.053*
C22	0.5053 (3)	0.1118 (3)	0.12736 (13)	0.0414 (7)
C15	0.2106 (2)	−0.0143 (3)	0.44110 (13)	0.0424 (7)
H15	0.1627	−0.0930	0.4408	0.051*
C20	0.5029 (2)	0.2266 (3)	0.22887 (14)	0.0410 (7)
H20	0.5319	0.2939	0.2629	0.049*
C23	0.4174 (3)	0.0305 (3)	0.12806 (13)	0.0457 (8)
H23	0.3865	−0.0331	0.0931	0.055*
C26	0.6246 (3)	0.1806 (5)	0.06639 (18)	0.0720 (12)
H26A	0.6056	0.2876	0.0670	0.108*
H26B	0.6391	0.1571	0.0256	0.108*
H26C	0.6857	0.1606	0.1013	0.108*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0421 (4)	0.0288 (3)	0.0284 (3)	0.0034 (3)	0.0165 (3)	0.0052 (3)
O3	0.0422 (12)	0.0378 (10)	0.0313 (10)	0.0025 (8)	0.0177 (9)	0.0018 (8)
O4	0.0505 (14)	0.0465 (11)	0.0335 (10)	−0.0113 (10)	0.0043 (10)	0.0158 (9)
O2	0.0459 (13)	0.0443 (10)	0.0261 (10)	−0.0015 (9)	0.0085 (9)	0.0007 (8)
N2	0.0369 (13)	0.0303 (10)	0.0229 (10)	0.0013 (9)	0.0111 (9)	0.0047 (8)
O1	0.0568 (15)	0.0421 (11)	0.0519 (12)	0.0192 (10)	0.0171 (11)	0.0056 (9)
N3	0.0391 (14)	0.0349 (11)	0.0330 (12)	0.0076 (10)	0.0156 (10)	0.0088 (9)
N1	0.0333 (14)	0.0305 (11)	0.0363 (13)	−0.0008 (10)	0.0083 (10)	0.0018 (9)
C11	0.0331 (15)	0.0287 (12)	0.0250 (12)	−0.0039 (11)	0.0094 (11)	−0.0006 (10)
C18	0.0321 (16)	0.0310 (13)	0.0339 (14)	−0.0072 (11)	0.0108 (12)	0.0003 (10)
C13	0.0353 (15)	0.0286 (12)	0.0228 (12)	0.0006 (11)	0.0108 (11)	0.0028 (9)
C10	0.0336 (15)	0.0283 (12)	0.0282 (13)	−0.0023 (11)	0.0113 (11)	−0.0012 (10)
C1	0.0249 (14)	0.0339 (13)	0.0228 (12)	−0.0027 (10)	0.0033 (10)	0.0022 (10)
C8	0.0355 (16)	0.0331 (13)	0.0323 (14)	0.0046 (11)	0.0145 (12)	0.0038 (11)
C19	0.0382 (17)	0.0325 (13)	0.0287 (14)	0.0069 (12)	0.0070 (12)	0.0057 (11)
C17	0.0277 (14)	0.0369 (13)	0.0220 (12)	−0.0031 (11)	0.0029 (10)	0.0009 (10)
C6	0.0246 (14)	0.0360 (13)	0.0262 (13)	0.0024 (11)	0.0066 (11)	0.0043 (10)
C9	0.0350 (16)	0.0328 (13)	0.0320 (14)	0.0012 (11)	0.0136 (12)	0.0034 (11)
O5	0.089 (2)	0.0627 (14)	0.0466 (13)	0.0304 (14)	0.0413 (13)	0.0104 (11)
C7	0.0301 (15)	0.0332 (13)	0.0292 (13)	0.0020 (11)	0.0099 (11)	0.0042 (10)
C12	0.0347 (16)	0.0289 (12)	0.0251 (13)	−0.0029 (11)	0.0057 (11)	0.0043 (10)
C16	0.0380 (16)	0.0322 (13)	0.0267 (13)	−0.0032 (11)	0.0076 (12)	0.0060 (10)
C2	0.0367 (17)	0.0378 (14)	0.0358 (15)	−0.0016 (12)	0.0083 (13)	0.0088 (12)
C14	0.0439 (18)	0.0400 (14)	0.0280 (14)	−0.0110 (13)	−0.0023 (12)	0.0029 (11)

C5	0.0344 (16)	0.0417 (15)	0.0334 (14)	0.0056 (12)	0.0102 (12)	−0.0001 (11)
C3	0.0363 (17)	0.0498 (16)	0.0250 (13)	−0.0067 (13)	0.0095 (12)	0.0083 (12)
C4	0.0393 (18)	0.0611 (18)	0.0259 (14)	0.0010 (14)	0.0134 (12)	−0.0010 (13)
C25	0.0487 (19)	0.0479 (16)	0.0231 (13)	0.0058 (14)	0.0069 (13)	0.0086 (11)
C24	0.0420 (18)	0.0426 (15)	0.0404 (16)	−0.0018 (13)	0.0081 (14)	0.0027 (13)
C21	0.0327 (17)	0.0575 (18)	0.0430 (17)	0.0041 (14)	0.0133 (14)	0.0133 (14)
C22	0.055 (2)	0.0394 (15)	0.0338 (15)	0.0207 (14)	0.0188 (14)	0.0103 (12)
C15	0.0464 (19)	0.0370 (14)	0.0399 (16)	−0.0170 (13)	0.0044 (14)	0.0069 (12)
C20	0.0431 (18)	0.0414 (15)	0.0373 (16)	−0.0006 (13)	0.0086 (14)	−0.0011 (12)
C23	0.059 (2)	0.0449 (16)	0.0297 (15)	−0.0013 (15)	0.0048 (14)	−0.0069 (12)
C26	0.065 (3)	0.100 (3)	0.065 (2)	0.041 (2)	0.042 (2)	0.040 (2)

Geometric parameters (Å, º)

S1—C10	1.753 (3)	C9—H9	0.96 (3)
S1—C12	1.777 (2)	O5—C22	1.375 (3)
O3—C11	1.206 (3)	O5—C26	1.385 (5)
O4—C16	1.365 (3)	C7—H7	1.00 (3)
O4—C25	1.431 (3)	C16—C15	1.395 (4)
O2—N1	1.232 (3)	C2—C3	1.384 (4)
N2—C11	1.385 (3)	C2—H2	0.9300
N2—C12	1.389 (3)	C14—C15	1.383 (4)
N2—C13	1.439 (3)	C14—H14	0.9300
O1—N1	1.226 (3)	C5—C4	1.377 (4)
N3—C12	1.267 (3)	C5—H5	0.9300
N3—C19	1.426 (3)	C3—C4	1.389 (4)
N1—C1	1.449 (3)	C3—H3	0.9300
C11—C10	1.490 (3)	C4—H4	0.9300
C18—C17	1.378 (3)	C25—H25A	0.9600
C18—C13	1.383 (4)	C25—H25B	0.9600
C18—H18	0.9300	C25—H25C	0.9600
C13—C14	1.382 (4)	C24—C23	1.388 (4)
C10—C9	1.336 (4)	C24—H24	0.9300
C1—C2	1.394 (3)	C21—C20	1.383 (4)
C1—C6	1.406 (3)	C21—C22	1.397 (4)
C8—C7	1.341 (3)	C21—H21	0.9300
C8—C9	1.438 (3)	C22—C23	1.365 (4)
C8—H8	0.94 (3)	C15—H15	0.9300
C19—C20	1.385 (4)	C20—H20	0.9300
C19—C24	1.386 (4)	C23—H23	0.9300
C17—C16	1.399 (4)	C26—H26A	0.9600
C17—H17	0.9300	C26—H26B	0.9600
C6—C5	1.399 (4)	C26—H26C	0.9600
C6—C7	1.465 (3)		
C10—S1—C12	91.41 (12)	O4—C16—C17	124.0 (2)
C16—O4—C25	116.7 (2)	C15—C16—C17	119.9 (2)
C11—N2—C12	116.9 (2)	C3—C2—C1	120.1 (3)

C11—N2—C13	120.9 (2)	C3—C2—H2	120.0
C12—N2—C13	122.1 (2)	C1—C2—H2	120.0
C12—N3—C19	116.0 (2)	C13—C14—C15	119.7 (2)
O1—N1—O2	122.5 (2)	C13—C14—H14	120.1
O1—N1—C1	118.3 (2)	C15—C14—H14	120.1
O2—N1—C1	119.2 (2)	C4—C5—C6	122.5 (3)
O3—C11—N2	124.6 (2)	C4—C5—H5	118.7
O3—C11—C10	125.5 (2)	C6—C5—H5	118.7
N2—C11—C10	109.9 (2)	C2—C3—C4	118.9 (2)
C17—C18—C13	120.5 (2)	C2—C3—H3	120.6
C17—C18—H18	119.7	C4—C3—H3	120.6
C13—C18—H18	119.8	C5—C4—C3	120.6 (3)
C14—C13—C18	120.5 (2)	C5—C4—H4	119.7
C14—C13—N2	120.5 (2)	C3—C4—H4	119.7
C18—C13—N2	119.0 (2)	O4—C25—H25A	109.5
C9—C10—C11	122.8 (2)	O4—C25—H25B	109.5
C9—C10—S1	126.1 (2)	H25A—C25—H25B	109.5
C11—C10—S1	111.07 (18)	O4—C25—H25C	109.5
C2—C1—C6	122.2 (2)	H25A—C25—H25C	109.5
C2—C1—N1	116.2 (2)	H25B—C25—H25C	109.5
C6—C1—N1	121.6 (2)	C19—C24—C23	120.0 (3)
C7—C8—C9	122.4 (3)	C19—C24—H24	120.0
C7—C8—H8	118.8	C23—C24—H24	120.0
C9—C8—H8	118.8	C20—C21—C22	118.3 (3)
C20—C19—C24	118.2 (3)	C20—C21—H21	120.8
C20—C19—N3	121.4 (2)	C22—C21—H21	120.8
C24—C19—N3	120.4 (3)	C23—C22—O5	115.8 (3)
C18—C17—C16	119.3 (2)	C23—C22—C21	119.9 (3)
C18—C17—H17	120.3	O5—C22—C21	124.3 (3)
C16—C17—H17	120.3	C14—C15—C16	120.0 (2)
C5—C6—C1	115.8 (2)	C14—C15—H15	120.0
C5—C6—C7	120.8 (2)	C16—C15—H15	120.0
C1—C6—C7	123.4 (2)	C21—C20—C19	122.3 (3)
C10—C9—C8	124.8 (3)	C21—C20—H20	118.8
C10—C9—H9	117.6	C19—C20—H20	118.8
C8—C9—H9	117.6	C22—C23—C24	121.1 (3)
C22—O5—C26	118.7 (3)	C22—C23—H23	119.5
C8—C7—C6	123.9 (3)	C24—C23—H23	119.5
C8—C7—H7	118.1	O5—C26—H26A	109.5
C6—C7—H7	118.0	O5—C26—H26B	109.5
N3—C12—N2	124.2 (2)	H26A—C26—H26B	109.5
N3—C12—S1	125.1 (2)	O5—C26—H26C	109.5
N2—C12—S1	110.65 (18)	H26A—C26—H26C	109.5
O4—C16—C15	116.1 (2)	H26B—C26—H26C	109.5

C12—N2—C11—O3	178.2 (2)	C11—N2—C12—N3	−177.1 (2)
C13—N2—C11—O3	1.4 (4)	C13—N2—C12—N3	−0.3 (4)
C12—N2—C11—C10	−3.3 (3)	C11—N2—C12—S1	2.9 (3)

C13—N2—C11—C10	179.8 (2)	C13—N2—C12—S1	179.67 (18)
C17—C18—C13—C14	0.7 (4)	C10—S1—C12—N3	178.9 (2)
C17—C18—C13—N2	179.1 (2)	C10—S1—C12—N2	−1.16 (19)
C11—N2—C13—C14	83.3 (3)	C25—O4—C16—C15	170.5 (3)
C12—N2—C13—C14	−93.4 (3)	C25—O4—C16—C17	−9.6 (4)
C11—N2—C13—C18	−95.1 (3)	C18—C17—C16—O4	178.6 (3)
C12—N2—C13—C18	88.2 (3)	C18—C17—C16—C15	−1.5 (4)
O3—C11—C10—C9	2.6 (4)	C6—C1—C2—C3	1.1 (4)
N2—C11—C10—C9	−175.9 (2)	N1—C1—C2—C3	178.8 (2)
O3—C11—C10—S1	−179.3 (2)	C18—C13—C14—C15	−0.3 (4)
N2—C11—C10—S1	2.3 (3)	N2—C13—C14—C15	−178.7 (3)
C12—S1—C10—C9	177.4 (3)	C1—C6—C5—C4	2.1 (4)
C12—S1—C10—C11	−0.63 (19)	C7—C6—C5—C4	−179.2 (3)
O1—N1—C1—C2	33.4 (4)	C1—C2—C3—C4	0.4 (4)
O2—N1—C1—C2	−145.6 (2)	C6—C5—C4—C3	−0.7 (5)
O1—N1—C1—C6	−148.8 (2)	C2—C3—C4—C5	−0.7 (4)
O2—N1—C1—C6	32.2 (4)	C20—C19—C24—C23	−0.4 (4)
C12—N3—C19—C20	81.3 (3)	N3—C19—C24—C23	−179.8 (2)
C12—N3—C19—C24	−99.3 (3)	C26—O5—C22—C23	172.6 (3)
C13—C18—C17—C16	0.2 (4)	C26—O5—C22—C21	−4.3 (4)
C2—C1—C6—C5	−2.3 (4)	C20—C21—C22—C23	3.7 (4)
N1—C1—C6—C5	−179.9 (2)	C20—C21—C22—O5	−179.4 (3)
C2—C1—C6—C7	179.1 (2)	C13—C14—C15—C16	−1.0 (5)
N1—C1—C6—C7	1.5 (4)	O4—C16—C15—C14	−178.1 (3)
C11—C10—C9—C8	175.7 (2)	C17—C16—C15—C14	1.9 (5)
S1—C10—C9—C8	−2.1 (4)	C22—C21—C20—C19	−1.4 (4)
C7—C8—C9—C10	−179.6 (3)	C24—C19—C20—C21	−0.3 (4)
C9—C8—C7—C6	176.6 (2)	N3—C19—C20—C21	179.2 (2)
C5—C6—C7—C8	26.7 (4)	O5—C22—C23—C24	178.5 (3)
C1—C6—C7—C8	−154.7 (3)	C21—C22—C23—C24	−4.4 (4)
C19—N3—C12—N2	179.4 (2)	C19—C24—C23—C22	2.7 (4)
C19—N3—C12—S1	−0.6 (4)		

Hydrogen-bond geometry (Å, º)

Cg3 is the centroid of the C13–C18 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···O3^{i}	1.00 (2)	2.55 (2)	3.197 (3)	122 (1)
C9—H9···O2^{ii}	0.97 (2)	2.58 (2)	3.400 (3)	142 (1)
C15—H15···O1^{iii}	0.93	2.59	3.286 (3)	132
C3—H3···*Cg*3^{iv}	0.93	2.80	3.560 (3)	140

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