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ISSN 2414-3146

1-(4-Methylbenzenesulfonyl)-1-phenyl-1*H*,2*H*-cyclobuta[*c*]quinoline

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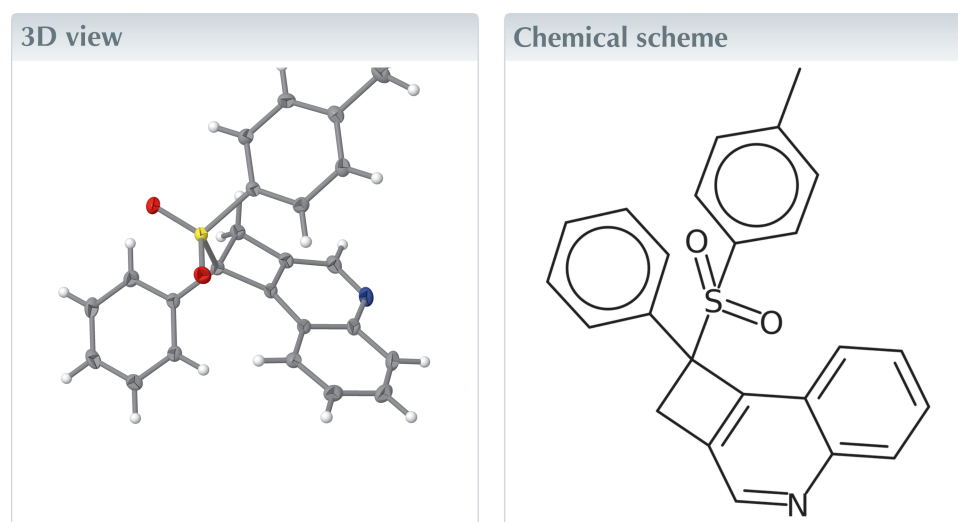
Received 12 November 2025

Accepted 13 November 2025

Edited by M. Bolte, Goethe-Universität Frankfurt, Germany

Keywords: crystal structure; hydrogen bridge; heterocycle; cyclobutene; 2 + 2 cycloaddition; 1,5-sulfonyl shift.**CCDC reference:** 2502744**Structural data:** full structural data are available from iucrdata.iucr.org

The title compound, C₂₄H₁₉NO₂S, forms strands along the *b*-axis direction *via* hydrogen bonds from the tolyl group to the sulfonyl oxygen atoms. The tricyclic framework is almost planar and the two six-membered aromatic substituents are nearly coparallel.



Structure description

The title compound, C₂₄H₁₉NO₂S (Fig. 1), was prepared in a larger project on indoloannulated heterocycles (Dassonneville *et al.*, 2023; Limbach *et al.*, 2018; Letessier *et al.*, 2013). It is an isomer and follow-up product of the recently reported *N*-propargyl-*N*-tosylaminotolane (Dassonneville *et al.*, 2025). The cyclobutene ring and the quinoline system include a dihedral angle of 5.04 (9)°, C11 [0.159 (2) Å] and C12 [0.026 (2) Å] lie below the quinoline plane. The interplanar angle between the quinoline system and the phenyl ring is 57.42 (6)°, the latter is almost parallel to the tolyl unit. The interplanar angle is only 6.03 (7)°. The bond angles in the cyclobutene unit are larger at the *sp*³-carbon atoms (C11–C3–C4: 94.75 (13)°, C3–C4–C12: 93.72 (13)°) than on the *sp*²-carbon atoms: C4–C12–C11: 86.19 (11)° and C12–C11–C3: 85.29 (11)°. The crystal packing features chains along the *b*-axis direction. The molecules are connected *via* hydrogen bonds (Table 1, Fig. 2) from the tolyl ring to the sulfonyl O atom, lengths are H23···O2: 2.52 Å and H24···O1: 2.47 Å, angles are C23–H23···O2: 161° and C24–H24···O1: 137°. A twofold screw axis relates the molecules geometrically.

Synthesis and crystallization

The title compound, C₂₄H₁₉NO₂S, appeared as by-product in low yield in the propargylation of 2-tosylaminotolane (Dassonneville *et al.*, 2025). A possible mechanistic pathway is given in Fig. 3. A base-catalyzed isomerization of the propargyl unit to an allenyl substituent followed by 2 + 2 cycloaddition of the outer double bond of the allene

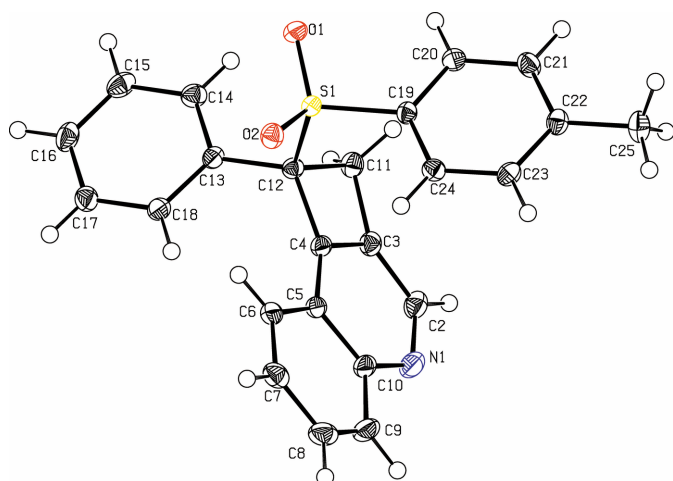


Figure 1
View the title compound. Displacement ellipsoids are drawn at the 50% probability level.

with the tolane triple bond generates a cyclobutene with concomitant closure of the quinoline ring. A supra-suprafacial 1,5-shift of the sulfonyl group from quinoline-N to a cyclobutene ring with aromatization of the pyridine ring gives the final compound. The compound crystallized from toluene solution as brownish crystals with m.p. = 426 K. The annotation of NMR signals follows IUPAC nomenclature. ¹H-NMR (400 MHz, CDCl₃): 8.66 (*s*, 1 H, 2-H quin); 8.20 (*dd*, *J* = 8 Hz, *J'* = 4 Hz), 8.16 (*dd*, *J* = 8 Hz, *J'* = 4 Hz) (5-H, 8-H quin), 7.80 (*ddd*, 1 H), 7.74 (*ddd*, 1 H) (6-H, 7-H, quin), 7.67–7.63 (*m*, 2 H, ph), 7.42–7.35 (*m*, 5 H, ph + tol), 7.09 (*d*, 2 H, 3-H, 5-H, tol), 4.20 (*d*, *J* = 16 Hz, CH₂), 3.77 (*d*, *J* = 16 Hz, CH₂), 2.37 (*s*, 3 H, CH₃). ¹³C-NMR (100 MHz, CDCl₃): 147.09 (C_q), 147.32 (C_q), 145.27 (C_q), 144.75 (CH, C-2 quin), 136.44 (C_q), 132.96 (C_q), 132.32 (C_q), 131.28 (CH, C-6 or C-7 quin), 130.11 (2 CH), 130.08 (2 CH), 129.22 (CH), 129.19 (2 CH), 129.02 (CH),

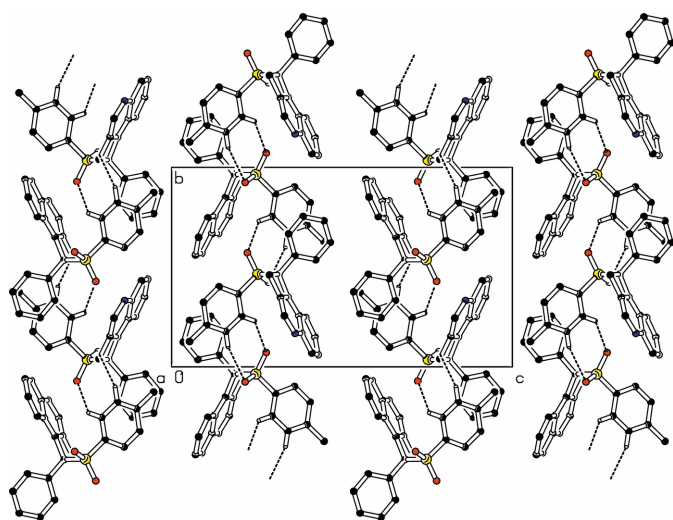


Figure 2
Part of the packing diagram. View along the *a*-axis direction. Hydrogen bonds are shown as dashed lines.

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

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
C23–H23···O2 ⁱ	0.95	2.52	3.431 (2)	161
C24–H24···O1 ⁱ	0.95	2.47	3.2357 (19)	137

Symmetry code: (i) $-x + \frac{3}{2}, y - \frac{1}{2}, -z + \frac{1}{2}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	C ₂₄ H ₁₉ NO ₂ S
<i>M_r</i>	385.46
Crystal system, space group	Monoclinic, <i>P</i> ₂ / <i>n</i>
Temperature (K)	120
<i>a</i> , <i>b</i> , <i>c</i> (Å)	7.5268 (3), 12.0672 (7), 20.6402 (9)
β (°)	92.740 (3)
<i>V</i> (Å ³)	1872.55 (16)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.19
Crystal size (mm)	0.44 × 0.36 × 0.18
Data collection	
Diffractometer	STOE <i>IPDS</i> 2T
Absorption correction	Integration (<i>X-RED3</i> ; Stoe & Cie, 2020)
<i>T_{min}</i> , <i>T_{max}</i>	0.933, 0.979
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	9143, 4455, 3856
<i>R_{int}</i>	0.022
(sin θ/λ) _{max} (Å ⁻¹)	0.660
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.042, 0.109, 1.08
No. of reflections	4455
No. of parameters	254
H-atom treatment	H-atom parameters constrained
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.49, –0.38

Computer programs 2.5.18.0 (Stoe & Cie, 2020), *SHELXT2014* (Sheldrick, 2015a), *SHELXL2019/2* (Sheldrick, 2015b) and *PLATON* (Spek, 2009).

128.52 (CH), 128.32 (2 CH), 124.33 (CH, C-7 or C-6 quin), 123.97 (C_q), 78.96 (C_q), 42.26 (CH₂), 21.66 (CH₃).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

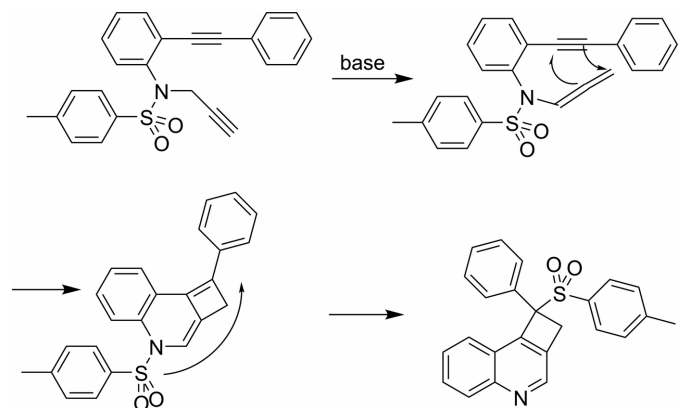


Figure 3
Possible synthetic mechanism.

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full crystallographic data

IUCrData (2025). **10**, x251019 [<https://doi.org/10.1107/S2414314625010193>]

1-(4-Methylbenzenesulfonyl)-1-phenyl-1*H*,2*H*-cyclobuta[*c*]quinoline

Dieter Schollmeyer, Benjamin Dassonneville and Heiner Detert

1-(4-Methylbenzenesulfonyl)-1-phenyl-1*H*,2*H*-cyclobuta[*c*]quinoline*Crystal data*

$C_{24}H_{19}NO_2S$	$F(000) = 808$
$M_r = 385.46$	$D_x = 1.367 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 7.5268 (3) \text{ \AA}$	Cell parameters from 12708 reflections
$b = 12.0672 (7) \text{ \AA}$	$\theta = 2.6\text{--}28.4^\circ$
$c = 20.6402 (9) \text{ \AA}$	$\mu = 0.19 \text{ mm}^{-1}$
$\beta = 92.740 (3)^\circ$	$T = 120 \text{ K}$
$V = 1872.55 (16) \text{ \AA}^3$	Block, colorless
$Z = 4$	$0.44 \times 0.36 \times 0.18 \text{ mm}$

Data collection

STOE IPDS 2T	4455 independent reflections
diffractometer	3856 reflections with $I > 2\sigma(I)$
Detector resolution: $6.67 \text{ pixels mm}^{-1}$	$R_{\text{int}} = 0.022$
rotation method, ω scans	$\theta_{\text{max}} = 28.0^\circ$, $\theta_{\text{min}} = 2.6^\circ$
Absorption correction: integration	$h = -9 \rightarrow 9$
(X-Red3; Stoe & Cie, 2020)	$k = -13 \rightarrow 15$
$T_{\text{min}} = 0.933$, $T_{\text{max}} = 0.979$	$l = -23 \rightarrow 27$
9143 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.042$	$w = 1/[\sigma^2(F_o^2) + (0.0478P)^2 + 1.4388P]$
$wR(F^2) = 0.109$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{\text{max}} = 0.001$
4455 reflections	$\Delta\rho_{\text{max}} = 0.49 \text{ e \AA}^{-3}$
254 parameters	$\Delta\rho_{\text{min}} = -0.38 \text{ e \AA}^{-3}$
0 restraints	
Primary atom site location: dual	

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. Hydrogen atoms were placed at calculated positions and were refined in the riding-model approximation with $C_{\text{aromatic}}\text{-H} = 0.95 \text{ \AA}$, $C_{\text{methyl}}\text{-H} = 0.98 \text{ \AA}$, $C_{\text{methylene}}\text{-H} = 0.99 \text{ \AA}$, and with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ for aromatic and methylene H atoms and with $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{C}_{\text{methyl}})$. The methyl group was allowed to rotate but not to tip.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.64207 (5)	0.46384 (3)	0.25290 (2)	0.01500 (11)
O1	0.63964 (16)	0.57122 (9)	0.22241 (5)	0.0202 (2)
N1	0.2289 (2)	0.16806 (12)	0.36221 (7)	0.0245 (3)
O2	0.80565 (15)	0.42439 (10)	0.28432 (5)	0.0199 (2)
C2	0.1616 (2)	0.25542 (14)	0.33105 (8)	0.0228 (3)
H2	0.039969	0.255983	0.316417	0.027*
C3	0.2704 (2)	0.34742 (14)	0.31963 (7)	0.0187 (3)
C4	0.4442 (2)	0.34911 (13)	0.34160 (7)	0.0165 (3)
C5	0.5253 (2)	0.25768 (13)	0.37323 (7)	0.0172 (3)
C6	0.7067 (2)	0.24665 (13)	0.39355 (7)	0.0190 (3)
H6	0.786202	0.306822	0.388467	0.023*
C7	0.7677 (2)	0.14939 (14)	0.42053 (8)	0.0231 (3)
H7	0.890248	0.141725	0.433003	0.028*
C8	0.6503 (3)	0.06065 (15)	0.42992 (8)	0.0267 (4)
H8	0.694212	-0.005968	0.449289	0.032*
C9	0.4743 (3)	0.06914 (14)	0.41153 (8)	0.0258 (4)
H9	0.396757	0.008686	0.418641	0.031*
C10	0.4059 (2)	0.16729 (13)	0.38190 (8)	0.0203 (3)
C11	0.2768 (2)	0.46028 (13)	0.28729 (8)	0.0190 (3)
H11A	0.198639	0.516693	0.305973	0.023*
H11B	0.262576	0.458325	0.239374	0.023*
C12	0.4775 (2)	0.46404 (12)	0.31482 (7)	0.0156 (3)
C13	0.5228 (2)	0.55765 (13)	0.36154 (7)	0.0164 (3)
C14	0.4825 (2)	0.66637 (14)	0.34362 (8)	0.0206 (3)
H14	0.427011	0.681116	0.302206	0.025*
C15	0.5227 (2)	0.75340 (14)	0.38585 (9)	0.0242 (3)
H15	0.497528	0.827501	0.372878	0.029*
C16	0.5998 (2)	0.73204 (15)	0.44701 (8)	0.0249 (4)
H16	0.625610	0.791420	0.476187	0.030*
C17	0.6390 (2)	0.62422 (15)	0.46546 (8)	0.0216 (3)
H17	0.691211	0.609713	0.507426	0.026*
C18	0.6024 (2)	0.53691 (13)	0.42282 (8)	0.0183 (3)
H18	0.631596	0.463158	0.435420	0.022*
C19	0.5675 (2)	0.36514 (13)	0.19515 (7)	0.0156 (3)
C20	0.4723 (2)	0.40126 (13)	0.13940 (8)	0.0191 (3)
H20	0.446551	0.477642	0.132914	0.023*
C21	0.4162 (2)	0.32307 (14)	0.09379 (8)	0.0208 (3)
H21	0.351596	0.346458	0.055557	0.025*
C22	0.4529 (2)	0.21033 (14)	0.10284 (8)	0.0188 (3)
C23	0.5476 (2)	0.17718 (13)	0.15898 (8)	0.0182 (3)
H23	0.572953	0.100793	0.165659	0.022*
C24	0.6058 (2)	0.25370 (13)	0.20536 (8)	0.0174 (3)
H24	0.670775	0.230324	0.243521	0.021*
C25	0.3904 (2)	0.12684 (15)	0.05270 (8)	0.0255 (4)
H25A	0.443051	0.143849	0.011332	0.038*

H25B	0.260469	0.129811	0.047153	0.038*
H25C	0.427041	0.052451	0.066930	0.038*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.01716 (18)	0.01263 (18)	0.01518 (18)	-0.00107 (13)	0.00034 (13)	-0.00060 (13)
O1	0.0275 (6)	0.0139 (5)	0.0194 (5)	-0.0026 (4)	0.0024 (4)	0.0008 (4)
N1	0.0271 (7)	0.0199 (7)	0.0269 (7)	-0.0069 (6)	0.0049 (6)	-0.0025 (6)
O2	0.0176 (5)	0.0206 (6)	0.0213 (5)	-0.0007 (4)	-0.0014 (4)	-0.0010 (5)
C2	0.0201 (8)	0.0236 (8)	0.0249 (8)	-0.0050 (6)	0.0026 (6)	-0.0039 (7)
C3	0.0200 (7)	0.0185 (8)	0.0178 (7)	-0.0012 (6)	0.0023 (6)	-0.0030 (6)
C4	0.0201 (7)	0.0146 (7)	0.0149 (7)	-0.0022 (6)	0.0033 (5)	-0.0015 (5)
C5	0.0234 (8)	0.0146 (7)	0.0139 (7)	-0.0017 (6)	0.0031 (6)	-0.0019 (5)
C6	0.0247 (8)	0.0170 (7)	0.0156 (7)	-0.0005 (6)	0.0013 (6)	-0.0008 (6)
C7	0.0295 (9)	0.0222 (8)	0.0176 (7)	0.0048 (7)	0.0011 (6)	-0.0007 (6)
C8	0.0413 (10)	0.0173 (8)	0.0218 (8)	0.0044 (7)	0.0044 (7)	0.0028 (6)
C9	0.0387 (10)	0.0141 (8)	0.0251 (8)	-0.0047 (7)	0.0067 (7)	-0.0005 (6)
C10	0.0292 (8)	0.0149 (7)	0.0172 (7)	-0.0032 (6)	0.0053 (6)	-0.0029 (6)
C11	0.0167 (7)	0.0191 (8)	0.0212 (7)	0.0006 (6)	-0.0008 (6)	-0.0014 (6)
C12	0.0166 (7)	0.0136 (7)	0.0165 (7)	0.0007 (5)	0.0010 (5)	0.0003 (6)
C13	0.0169 (7)	0.0153 (7)	0.0173 (7)	-0.0017 (5)	0.0031 (5)	-0.0015 (6)
C14	0.0236 (8)	0.0172 (8)	0.0213 (7)	0.0020 (6)	0.0030 (6)	0.0007 (6)
C15	0.0281 (9)	0.0146 (8)	0.0305 (9)	0.0007 (6)	0.0074 (7)	-0.0010 (7)
C16	0.0281 (9)	0.0221 (9)	0.0251 (8)	-0.0061 (7)	0.0071 (7)	-0.0094 (7)
C17	0.0225 (8)	0.0245 (8)	0.0181 (7)	-0.0044 (6)	0.0032 (6)	-0.0025 (6)
C18	0.0197 (7)	0.0164 (7)	0.0189 (7)	-0.0012 (6)	0.0025 (6)	-0.0002 (6)
C19	0.0169 (7)	0.0144 (7)	0.0157 (7)	-0.0003 (5)	0.0008 (5)	-0.0021 (6)
C20	0.0223 (8)	0.0152 (7)	0.0195 (7)	0.0013 (6)	-0.0008 (6)	0.0010 (6)
C21	0.0235 (8)	0.0210 (8)	0.0176 (7)	0.0029 (6)	-0.0036 (6)	0.0001 (6)
C22	0.0165 (7)	0.0199 (8)	0.0201 (7)	-0.0009 (6)	0.0019 (6)	-0.0040 (6)
C23	0.0177 (7)	0.0144 (7)	0.0226 (7)	0.0009 (5)	0.0024 (6)	-0.0012 (6)
C24	0.0176 (7)	0.0167 (7)	0.0178 (7)	0.0021 (5)	0.0004 (5)	0.0009 (6)
C25	0.0262 (8)	0.0250 (9)	0.0247 (8)	0.0000 (7)	-0.0035 (7)	-0.0083 (7)

Geometric parameters (Å, °)

S1—O1	1.4402 (12)	C13—C14	1.393 (2)
S1—O2	1.4446 (11)	C13—C18	1.396 (2)
S1—C19	1.7579 (15)	C14—C15	1.389 (2)
S1—C12	1.8219 (15)	C14—H14	0.9500
N1—C2	1.323 (2)	C15—C16	1.388 (3)
N1—C10	1.374 (2)	C15—H15	0.9500
C2—C3	1.406 (2)	C16—C17	1.384 (2)
C2—H2	0.9500	C16—H16	0.9500
C3—C4	1.364 (2)	C17—C18	1.392 (2)
C3—C11	1.518 (2)	C17—H17	0.9500
C4—C5	1.406 (2)	C18—H18	0.9500

C4—C12	1.518 (2)	C19—C24	1.389 (2)
C5—C6	1.415 (2)	C19—C20	1.396 (2)
C5—C10	1.430 (2)	C20—C21	1.384 (2)
C6—C7	1.369 (2)	C20—H20	0.9500
C6—H6	0.9500	C21—C22	1.399 (2)
C7—C8	1.408 (3)	C21—H21	0.9500
C7—H7	0.9500	C22—C23	1.390 (2)
C8—C9	1.365 (3)	C22—C25	1.503 (2)
C8—H8	0.9500	C23—C24	1.386 (2)
C9—C10	1.418 (2)	C23—H23	0.9500
C9—H9	0.9500	C24—H24	0.9500
C11—C12	1.589 (2)	C25—H25A	0.9800
C11—H11A	0.9900	C25—H25B	0.9800
C11—H11B	0.9900	C25—H25C	0.9800
C12—C13	1.514 (2)		
O1—S1—O2	119.04 (7)	C4—C12—S1	112.56 (10)
O1—S1—C19	108.44 (7)	C11—C12—S1	114.56 (10)
O2—S1—C19	108.59 (7)	C14—C13—C18	119.23 (14)
O1—S1—C12	108.09 (7)	C14—C13—C12	119.61 (14)
O2—S1—C12	106.19 (7)	C18—C13—C12	121.15 (14)
C19—S1—C12	105.71 (7)	C15—C14—C13	120.48 (15)
C2—N1—C10	119.52 (14)	C15—C14—H14	119.8
N1—C2—C3	119.83 (15)	C13—C14—H14	119.8
N1—C2—H2	120.1	C16—C15—C14	119.97 (16)
C3—C2—H2	120.1	C16—C15—H15	120.0
C4—C3—C2	120.88 (15)	C14—C15—H15	120.0
C4—C3—C11	94.75 (13)	C17—C16—C15	119.95 (15)
C2—C3—C11	144.35 (15)	C17—C16—H16	120.0
C3—C4—C5	122.04 (15)	C15—C16—H16	120.0
C3—C4—C12	93.72 (13)	C16—C17—C18	120.30 (15)
C5—C4—C12	144.13 (14)	C16—C17—H17	119.8
C4—C5—C6	127.03 (14)	C18—C17—H17	119.8
C4—C5—C10	113.29 (14)	C17—C18—C13	120.04 (15)
C6—C5—C10	119.62 (15)	C17—C18—H18	120.0
C7—C6—C5	120.10 (15)	C13—C18—H18	120.0
C7—C6—H6	120.0	C24—C19—C20	121.45 (14)
C5—C6—H6	120.0	C24—C19—S1	119.72 (12)
C6—C7—C8	120.50 (16)	C20—C19—S1	118.82 (12)
C6—C7—H7	119.8	C21—C20—C19	118.39 (15)
C8—C7—H7	119.8	C21—C20—H20	120.8
C9—C8—C7	120.81 (16)	C19—C20—H20	120.8
C9—C8—H8	119.6	C20—C21—C22	121.36 (15)
C7—C8—H8	119.6	C20—C21—H21	119.3
C8—C9—C10	120.68 (16)	C22—C21—H21	119.3
C8—C9—H9	119.7	C23—C22—C21	118.75 (14)
C10—C9—H9	119.7	C23—C22—C25	120.80 (15)
N1—C10—C9	117.39 (15)	C21—C22—C25	120.45 (15)

N1—C10—C5	124.33 (15)	C24—C23—C22	121.10 (15)
C9—C10—C5	118.27 (16)	C24—C23—H23	119.4
C3—C11—C12	85.29 (11)	C22—C23—H23	119.4
C3—C11—H11A	114.4	C23—C24—C19	118.94 (14)
C12—C11—H11A	114.4	C23—C24—H24	120.5
C3—C11—H11B	114.4	C19—C24—H24	120.5
C12—C11—H11B	114.4	C22—C25—H25A	109.5
H11A—C11—H11B	111.6	C22—C25—H25B	109.5
C13—C12—C4	119.07 (13)	H25A—C25—H25B	109.5
C13—C12—C11	115.51 (12)	C22—C25—H25C	109.5
C4—C12—C11	86.19 (11)	H25A—C25—H25C	109.5
C13—C12—S1	107.93 (10)	H25B—C25—H25C	109.5
C10—N1—C2—C3	-1.4 (2)	C19—S1—C12—C13	-173.08 (10)
N1—C2—C3—C4	-1.5 (2)	O1—S1—C12—C4	169.44 (10)
N1—C2—C3—C11	176.2 (2)	O2—S1—C12—C4	-61.76 (12)
C2—C3—C4—C5	3.6 (2)	C19—S1—C12—C4	53.49 (12)
C11—C3—C4—C5	-175.11 (14)	O1—S1—C12—C11	73.08 (12)
C2—C3—C4—C12	-179.50 (15)	O2—S1—C12—C11	-158.12 (11)
C11—C3—C4—C12	1.81 (12)	C19—S1—C12—C11	-42.87 (12)
C3—C4—C5—C6	174.77 (15)	C4—C12—C13—C14	-153.41 (14)
C12—C4—C5—C6	0.0 (3)	C11—C12—C13—C14	-52.97 (19)
C3—C4—C5—C10	-2.5 (2)	S1—C12—C13—C14	76.70 (16)
C12—C4—C5—C10	-177.23 (19)	C4—C12—C13—C18	25.7 (2)
C4—C5—C6—C7	-176.19 (15)	C11—C12—C13—C18	126.14 (15)
C10—C5—C6—C7	0.9 (2)	S1—C12—C13—C18	-104.18 (15)
C5—C6—C7—C8	-1.7 (2)	C18—C13—C14—C15	0.8 (2)
C6—C7—C8—C9	0.9 (3)	C12—C13—C14—C15	179.89 (15)
C7—C8—C9—C10	0.6 (3)	C13—C14—C15—C16	-1.6 (3)
C2—N1—C10—C9	-176.19 (15)	C14—C15—C16—C17	1.0 (3)
C2—N1—C10—C5	2.4 (2)	C15—C16—C17—C18	0.3 (3)
C8—C9—C10—N1	177.31 (15)	C16—C17—C18—C13	-1.2 (2)
C8—C9—C10—C5	-1.4 (2)	C14—C13—C18—C17	0.6 (2)
C4—C5—C10—N1	-0.5 (2)	C12—C13—C18—C17	-178.52 (14)
C6—C5—C10—N1	-177.98 (14)	O1—S1—C19—C24	160.91 (12)
C4—C5—C10—C9	178.11 (14)	O2—S1—C19—C24	30.22 (15)
C6—C5—C10—C9	0.6 (2)	C12—S1—C19—C24	-83.38 (14)
C4—C3—C11—C12	-1.74 (12)	O1—S1—C19—C20	-18.36 (15)
C2—C3—C11—C12	-179.8 (2)	O2—S1—C19—C20	-149.06 (12)
C3—C4—C12—C13	115.45 (14)	C12—S1—C19—C20	97.34 (13)
C5—C4—C12—C13	-69.0 (3)	C24—C19—C20—C21	-0.1 (2)
C3—C4—C12—C11	-1.73 (12)	S1—C19—C20—C21	179.12 (12)
C5—C4—C12—C11	173.8 (2)	C19—C20—C21—C22	0.2 (2)
C3—C4—C12—S1	-116.78 (11)	C20—C21—C22—C23	0.0 (2)
C5—C4—C12—S1	58.8 (3)	C20—C21—C22—C25	179.90 (15)
C3—C11—C12—C13	-118.96 (13)	C21—C22—C23—C24	-0.2 (2)
C3—C11—C12—C4	1.56 (11)	C25—C22—C23—C24	179.92 (15)
C3—C11—C12—S1	114.66 (11)	C22—C23—C24—C19	0.2 (2)

O1—S1—C12—C13	-57.12 (12)	C20—C19—C24—C23	0.0 (2)
O2—S1—C12—C13	71.67 (11)	S1—C19—C24—C23	-179.29 (12)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C23—H23···O2 ⁱ	0.95	2.52	3.431 (2)	161
C24—H24···O1 ⁱ	0.95	2.47	3.2357 (19)	137

Symmetry code: (i) $-x+3/2, y-1/2, -z+1/2$.