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cis-1-Ethyl-4,4,10-trimethyl-2-tosyl-1,2,3,3a,4,11b-hexahydro-11*H*-pyrrolo-[3,4-*c*]pyrano[5,6-*c*]quinolin-11-one

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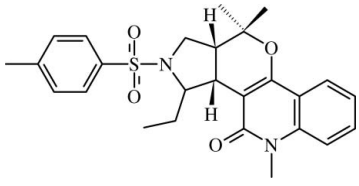
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.059; wR factor = 0.163; data-to-parameter ratio = 21.0.

The molecule of the title compound, $C_{26}H_{30}N_2O_4S$, adopts a folded conformation, with the sulfonyl-bound benzene ring lying over the pyridinone ring [centroid-to-centroid distance = 3.893 (1) Å], forming a dihedral angle of 23.87 (5)°. The pyrrolidine ring adopts a twist conformation and the dihydropyran ring is in a half-chair conformation. The pyrrolidine and dihydropyran rings are *cis*-fused. The sulfonyl group has a distorted tetrahedral geometry. In the crystal structure, the molecules are linked into a centrosymmetric $R_2^2(12)$ dimer by C—H···O hydrogen bonds. The dimers are cross-linked into a sheet parallel to the *bc* plane *via* C—H···π interactions involving the benzene ring of the quinolinone ring system. The ethyl group is disordered over two positions; the site-occupancy factors are *ca* 0.8 and 0.2.

Related literature

The structure of the title molecule is quite similar to that of 6,6-dimethyl-4-tosylpyrrolo[3,4-*c*]pyrano[5,6-*c*]-1-methylquinolin-2-one (Chinnakali *et al.*, 2007). For biological activities of pyranoquinolinones, see: Butenschön *et al.* (2001); Edwards *et al.* (1999); Hanawa *et al.* (2004); Kamikawa *et al.* (1996); Keenan (1994); Wasserman (1995). For ring-puckering parameters, see: Cremer & Pople (1975). For asymmetry parameters, see: Duax *et al.* (1976).



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Experimental

Crystal data

$C_{26}H_{30}N_2O_4S$
M_r = 466.58
Monoclinic, $P2_1/c$
a = 10.4111 (2) Å
b = 13.8576 (2) Å
c = 18.0460 (3) Å
β = 117.834 (1)°
V = 2302.33 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.18 mm^{-1}
T = 100.0 (1) K
0.52 × 0.43 × 0.33 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.874, T_{max} = 0.944
28627 measured reflections
6709 independent reflections
4846 reflections with $I > 2\sigma(I)$
R_{int} = 0.058

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.163
S = 1.03
6709 reflections
319 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.85 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

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

*Cg*1 is the centroid of the C17–C22 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O1^{i}	0.98	2.48	3.282 (2)	139
C4—H4···O4	0.98	2.38	2.974 (2)	118
C25*A*—H25*A*···*Cg*1^{ii}	0.97	2.87	3.706 (3)	145

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2214).

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supplementary materials

Acta Cryst. (2007). E**63**, o4491-o4492 [**doi:10.1107/S1600536807053263**]

cis-1-Ethyl-4,4,10-trimethyl-2-tosyl-1,2,3,3a,4,11b-hexahydro-11*H*-pyrrolo[3,4-*c*]pyrano[5,6-*c*]quinolin-11-one

K. Chinnakali, D. Sudha, M. Jayagopi, R. Raghunathan and H.-K. Fun

Comment

Some pyranoquinolone derivatives exhibit anti-inflammatory activity (Keenan, 1994; Wasserman 1995). Pyranoquinolone alkaloids exhibit photo-activated antimicrobial activity (Hanawa *et al.*, 2004) and SRS-A antagonist action (Kamikawa *et al.*, 1996). Pyranoquinolinones act as blockers of the voltage-gated potassium channel Kv1.3 (Butenschön *et al.*, 2001). 2*H*-pyrano[3,2-*g*]quinolin-2-one derivatives are found to modulate the transcriptional activity of the human androgen receptor (Edwards *et al.*, 1999). We report here the crystal structure of the title compound, a pyranoquinolinone derivative.

Bond lengths and angles in the title molecule (Fig. 1) are comparable to those observed in a related compound, 6,6-dimethyl-4-tosylpyrrolo[3,4-*c*]pyrano[5,6-*c*]-1- methylquinolin-2-one hemihydrate (Chinnakali *et al.*, 2007).

The pyrrolidine ring adopts a twist conformation, with the local twofold rotation axis passing through atom N1 and the mid-point of the opposite bond C2—C3; the asymmetry parameter (Duax *et al.*, 1976) ΔC_2[C2—C3] is 2.3 (2)°, and the puckering parameters (Cremer & Pople, 1975) are q_2 = 0.370 (2) Å and φ = 92.2 (3)°. The tosyl group is attached to the pyrrolidine ring in a biaxial position. The dihydropyran ring is in a half-chair conformation, with a local pseudo-twofold rotation axis running through the midpoints of the C2—C5 and C6—C7 bonds. The puckering parameters Q, θ and φ, and the smallest displacement asymmetry parameter ΔC_2[C2—C5] are 0.438 (2) Å, 50.6 (3)°, 87.1 (3)° and 4.6 (3)°, respectively. The pyrrolidine ring is *cis*-fused to the dihydropyran ring. The quinolinone ring system is planar, with an r.m.s. deviation of 0.030 Å, and atoms O4 and C24 deviating from the mean plane by 0.171 (2) and 0.084 (3) Å, respectively.

As expected, the sulfonyl group has a distorted tetrahedral geometry, with the O1—S1—O2 [119.40 (9)°] angle deviating significantly from the ideal tetrahedral value. The molecule is in a folded conformation, with the sulfonyl-bound benzene ring lying over the pyridinone ring. The centroid-centroid distance [3.893 (1) Å] and the dihedral angle [23.87 (5)°] between the two rings indicate the presence of weak π–π interactions between them.

In the crystal structure, centrosymmetrically related molecules are linked by a pair of C2—H2···O1^{i} hydrogen bonds (Table 1) into a $R_2^2(12)$ dimer. The dimers are linked into a sheet parallel to the *bc* plane (Fig. 2) *via* C25A—H25A···π interactions involving the C17–C22 ring (centroid *Cg*1) of the molecule at (1 − *x*, −1/2 + *y*, 1/2 − *z*).

Experimental

To a solution of 1-methylquinoline-2,4-dione (1 mmol) in dry toluene (20 ml), 2-[*N*-(3-methylbut-2-enyl)-*N*-tosylamino]butanal (1 mmol) and a catalytic amount of the base ethylenediamine-*N*,*N*'-diacetate (EDDA) were added and the reaction mixture was refluxed for 12 h. After completion of the reaction, the solvent was evaporated under reduced pressure and the crude product was chromatographed using a hexane–ethyl acetate (8:2 *v*/*v*) mixture to obtain the title compound. The compound was recrystallized from ethyl acetate solution by slow evaporation.

Refinement

The ethyl group is disordered over two orientations (C25A,C26A/C25B,C26B) with refined occupancies of 0.760 (5) and 0.240 (5). The corresponding C—C distances in the disordered components were restrained to be equal. H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93–0.98 Å. The U_{iso} values were set equal to $1.5U_{eq}$ of the carrier atom for methyl H atoms and $1.2U_{eq}$ for the remaining H atoms. A rotating group model was used for the methyl groups attached to aromatic rings.

Figures

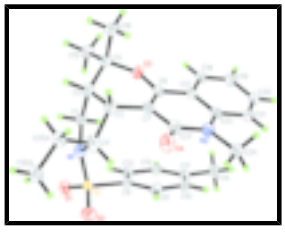


Fig. 1. The molecular structure of the title compound. Displacement ellipsoids are drawn at the 80% probability level. Only one disorder component is shown.

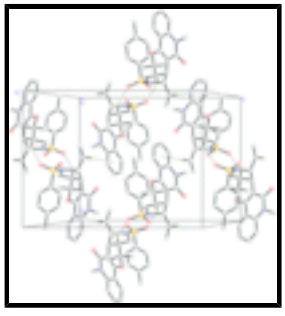


Fig. 2. View of a hydrogen-bonded sheet in the title compound. Dashed and dotted lines indicate C—H···O and C—H···π interactions, respectively. For the sake of clarity, H atoms not involved in the interactions have been omitted. Only one disorder component is shown.

cis-1-Ethyl-4,4,10-trimethyl-2-tosyl-1,2,3,3a,4,11*b*-hexahydro- 11*H*-pyrrolo[3,4-*c*]pyrano[5,6-*c*]quinolin-11-one

Crystal data

$C_{26}H_{30}N_2O_4S$	F_{000} = 992
M_r = 466.58	D_x = 1.346 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 6924 reflections
a = 10.4111 (2) Å	θ = 2.2–28.4º
b = 13.8576 (2) Å	μ = 0.18 mm^{-1}
c = 18.0460 (3) Å	T = 100.0 (1) K
β = 117.834 (1)º	Block, light yellow
V = 2302.33 (7) Å^3	0.52 × 0.43 × 0.33 mm
Z = 4	

Data collection

Bruker SMART APEXII CCD area-detector	6709 independent reflections

diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

Detector resolution: 8.33 pixels mm^{-1}

T = 100.0(1) K

ω scans

Absorption correction: multi-scan (SADABS; Bruker, 2005)

T_{min} = 0.874, T_{max} = 0.944

28627 measured reflections

4846 reflections with $I > 2\sigma(I)$

R_{int} = 0.058

θ_{max} = 30.1º

θ_{min} = 2.0º

$h = -14 \rightarrow 14$

$k = -15 \rightarrow 19$

$l = -25 \rightarrow 24$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.059

$wR(F^2)$ = 0.163

S = 1.03

6709 reflections

319 parameters

2 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0874P)^2 + 0.4457P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.001

$\Delta\rho_{max}$ = 0.85 e $Å^{-3}$

$\Delta\rho_{min}$ = −0.43 e $Å^{-3}$

Extinction correction: none

Special details

Experimental. The low-temparture data was collected with the Oxford Cyrosystem Cobra low-temperature attachment.

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.

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
S1	0.21372 (5)	0.08412 (3)	0.39792 (3)	0.02235 (13)	
O1	0.24491 (14)	0.04611 (10)	0.47870 (8)	0.0265 (3)	
O2	0.10426 (14)	0.03882 (10)	0.32371 (8)	0.0309 (3)	
O3	0.60238 (13)	0.32271 (10)	0.44037 (8)	0.0258 (3)	
O4	0.25960 (15)	0.22331 (11)	0.16712 (8)	0.0316 (3)	
N1	0.36407 (16)	0.07947 (11)	0.39179 (9)	0.0225 (3)	

N2	0.25256 (16)	0.37742 (12)	0.20890 (9)	0.0238 (3)	
C1	0.49235 (19)	0.12860 (14)	0.45792 (11)	0.0233 (4)	
H1A	0.5415	0.0874	0.5067	0.028*	
H1B	0.4646	0.1882	0.4748	0.028*	
C2	0.5894 (2)	0.14873 (14)	0.41714 (11)	0.0256 (4)	
H2	0.6491	0.0915	0.4237	0.031*	
C3	0.4814 (2)	0.16080 (14)	0.32352 (11)	0.0260 (4)	
H3	0.5295	0.1451	0.2896	0.031*	
C4	0.3652 (2)	0.08486 (14)	0.30939 (11)	0.0292 (4)	
H4	0.2700	0.1024	0.2635	0.035*	0.760 (5)
H4B	0.2776	0.1202	0.2762	0.035*	0.240 (5)
C5	0.68972 (19)	0.23514 (15)	0.45482 (12)	0.0276 (4)	
C6	0.48668 (18)	0.33451 (14)	0.36317 (11)	0.0224 (4)	
C7	0.42612 (19)	0.26299 (14)	0.30625 (11)	0.0229 (4)	
C8	0.16642 (18)	0.20637 (13)	0.39735 (11)	0.0212 (4)	
C9	0.09429 (19)	0.25587 (15)	0.32132 (11)	0.0252 (4)	
H9	0.0673	0.2241	0.2708	0.030*	
C10	0.06369 (19)	0.35297 (15)	0.32241 (11)	0.0255 (4)	
H10	0.0164	0.3864	0.2720	0.031*	
C11	0.10221 (19)	0.40159 (14)	0.39735 (12)	0.0238 (4)	
C12	0.17227 (18)	0.35032 (14)	0.47219 (11)	0.0233 (4)	
H12	0.1971	0.3817	0.5226	0.028*	
C13	0.20556 (19)	0.25356 (14)	0.47281 (10)	0.0219 (4)	
H13	0.2537	0.2204	0.5233	0.026*	
C14	0.0690 (2)	0.50723 (15)	0.39761 (13)	0.0346 (5)	
H14A	0.0508	0.5355	0.3450	0.052*	
H14B	0.1502	0.5389	0.4423	0.052*	
H14C	−0.0154	0.5147	0.4057	0.052*	
C15	0.7767 (2)	0.22697 (16)	0.54924 (12)	0.0322 (5)	
H15A	0.7118	0.2179	0.5728	0.048*	
H15B	0.8319	0.2849	0.5714	0.048*	
H15C	0.8414	0.1728	0.5633	0.048*	
C16	0.7889 (2)	0.24952 (18)	0.41481 (14)	0.0376 (5)	
H16A	0.8506	0.3043	0.4398	0.056*	
H16B	0.7311	0.2604	0.3558	0.056*	
H16C	0.8476	0.1930	0.4237	0.056*	
C17	0.43063 (18)	0.43151 (14)	0.34636 (11)	0.0215 (4)	
C18	0.4934 (2)	0.50710 (15)	0.40380 (11)	0.0259 (4)	
H18	0.5740	0.4948	0.4551	0.031*	
C19	0.4376 (2)	0.59907 (15)	0.38551 (12)	0.0291 (4)	
H19	0.4804	0.6488	0.4239	0.035*	
C20	0.3159 (2)	0.61680 (15)	0.30867 (12)	0.0280 (4)	
H20	0.2766	0.6786	0.2965	0.034*	
C21	0.2532 (2)	0.54446 (14)	0.25068 (11)	0.0261 (4)	
H21	0.1727	0.5578	0.1996	0.031*	
C22	0.30974 (18)	0.45094 (14)	0.26793 (11)	0.0223 (4)	
C23	0.3089 (2)	0.28460 (14)	0.22321 (11)	0.0249 (4)	
C24	0.1320 (2)	0.39954 (15)	0.12554 (11)	0.0283 (4)	
H24A	0.0997	0.3412	0.0934	0.042*	

H24B	0.1646	0.4443	0.0973	0.042*	
H24C	0.0532	0.4275	0.1317	0.042*	
C25A	0.4228 (3)	−0.0123 (2)	0.29271 (17)	0.0268 (7)	0.760 (5)
H25A	0.4308	−0.0063	0.2415	0.032*	0.760 (5)
H25B	0.5194	−0.0241	0.3382	0.032*	0.760 (5)
C26A	0.3273 (3)	−0.0979 (2)	0.28484 (17)	0.0316 (7)	0.760 (5)
H26A	0.3686	−0.1552	0.2747	0.047*	0.760 (5)
H26B	0.2321	−0.0876	0.2390	0.047*	0.760 (5)
H26C	0.3205	−0.1054	0.3358	0.047*	0.760 (5)
C25B	0.3309 (9)	−0.0119 (5)	0.2635 (4)	0.026 (2)	0.240 (5)
H25C	0.2400	−0.0377	0.2576	0.032*	0.240 (5)
H25D	0.3237	−0.0046	0.2083	0.032*	0.240 (5)
C26B	0.4553 (8)	−0.0771 (6)	0.3171 (5)	0.027 (2)	0.240 (5)
H26D	0.4402	−0.1395	0.2914	0.041*	0.240 (5)
H26E	0.4609	−0.0832	0.3715	0.041*	0.240 (5)
H26F	0.5443	−0.0501	0.3226	0.041*	0.240 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0256 (2)	0.0191 (2)	0.0208 (2)	−0.00014 (17)	0.00949 (17)	−0.00027 (17)
O1	0.0326 (7)	0.0232 (7)	0.0264 (7)	0.0026 (6)	0.0160 (6)	0.0050 (5)
O2	0.0288 (7)	0.0279 (8)	0.0293 (7)	−0.0029 (6)	0.0080 (6)	−0.0069 (6)
O3	0.0232 (6)	0.0245 (7)	0.0237 (6)	0.0032 (5)	0.0060 (5)	0.0050 (5)
O4	0.0423 (8)	0.0292 (8)	0.0215 (6)	0.0011 (6)	0.0136 (6)	−0.0016 (6)
N1	0.0275 (7)	0.0218 (8)	0.0174 (7)	0.0012 (6)	0.0099 (6)	−0.0003 (6)
N2	0.0244 (7)	0.0260 (9)	0.0198 (7)	−0.0011 (6)	0.0094 (6)	0.0018 (6)
C1	0.0259 (8)	0.0226 (10)	0.0200 (8)	0.0003 (7)	0.0097 (7)	0.0018 (7)
C2	0.0287 (9)	0.0242 (10)	0.0263 (9)	0.0070 (8)	0.0149 (8)	0.0049 (7)
C3	0.0319 (9)	0.0276 (11)	0.0230 (8)	0.0069 (8)	0.0167 (8)	0.0042 (7)
C4	0.0464 (11)	0.0250 (11)	0.0200 (8)	−0.0038 (9)	0.0187 (8)	−0.0016 (7)
C5	0.0231 (8)	0.0275 (11)	0.0319 (10)	0.0062 (8)	0.0126 (8)	0.0069 (8)
C6	0.0207 (8)	0.0252 (10)	0.0221 (8)	0.0005 (7)	0.0107 (7)	0.0069 (7)
C7	0.0254 (8)	0.0233 (10)	0.0234 (8)	0.0005 (7)	0.0143 (7)	0.0038 (7)
C8	0.0224 (8)	0.0195 (9)	0.0214 (8)	0.0012 (7)	0.0099 (7)	0.0026 (7)
C9	0.0249 (9)	0.0285 (11)	0.0198 (8)	0.0033 (8)	0.0086 (7)	0.0012 (7)
C10	0.0257 (8)	0.0281 (11)	0.0225 (8)	0.0046 (8)	0.0112 (7)	0.0077 (7)
C11	0.0204 (8)	0.0239 (10)	0.0284 (9)	0.0005 (7)	0.0125 (7)	0.0028 (7)
C12	0.0243 (8)	0.0232 (10)	0.0220 (8)	−0.0009 (7)	0.0104 (7)	−0.0021 (7)
C13	0.0232 (8)	0.0228 (10)	0.0179 (8)	−0.0004 (7)	0.0080 (6)	0.0017 (7)
C14	0.0391 (11)	0.0237 (11)	0.0366 (11)	0.0042 (9)	0.0141 (9)	0.0026 (9)
C15	0.0256 (9)	0.0325 (12)	0.0306 (10)	0.0044 (8)	0.0065 (8)	0.0078 (9)
C16	0.0269 (10)	0.0438 (14)	0.0459 (12)	0.0022 (9)	0.0202 (9)	0.0074 (10)
C17	0.0210 (8)	0.0219 (10)	0.0228 (8)	−0.0001 (7)	0.0113 (7)	0.0042 (7)
C18	0.0246 (8)	0.0264 (11)	0.0241 (8)	−0.0014 (8)	0.0092 (7)	0.0047 (8)
C19	0.0293 (9)	0.0272 (11)	0.0278 (9)	−0.0015 (8)	0.0107 (8)	0.0019 (8)
C20	0.0285 (9)	0.0242 (10)	0.0297 (9)	0.0016 (8)	0.0122 (8)	0.0052 (8)
C21	0.0238 (8)	0.0272 (11)	0.0241 (9)	0.0020 (8)	0.0086 (7)	0.0070 (8)

C22	0.0221 (8)	0.0237 (10)	0.0226 (8)	−0.0029 (7)	0.0116 (7)	0.0024 (7)
C23	0.0296 (9)	0.0259 (10)	0.0228 (8)	0.0001 (8)	0.0153 (7)	0.0035 (7)
C24	0.0256 (9)	0.0340 (12)	0.0212 (8)	0.0024 (8)	0.0075 (7)	0.0014 (8)
C25A	0.0324 (16)	0.0238 (16)	0.0284 (13)	−0.0023 (12)	0.0176 (13)	−0.0056 (11)
C26A	0.0366 (15)	0.0271 (16)	0.0337 (14)	−0.0033 (11)	0.0187 (12)	−0.0077 (11)
C25B	0.018 (4)	0.039 (5)	0.017 (3)	−0.007 (3)	0.004 (3)	−0.001 (3)
C26B	0.034 (4)	0.029 (5)	0.023 (4)	−0.003 (4)	0.017 (3)	−0.007 (3)

Geometric parameters (Å, °)

S1—O2	1.4356 (13)	C12—C13	1.384 (3)
S1—O1	1.4374 (13)	C12—H12	0.93
S1—N1	1.6212 (16)	C13—H13	0.93
S1—C8	1.7629 (19)	C14—H14A	0.96
O3—C6	1.361 (2)	C14—H14B	0.96
O3—C5	1.465 (2)	C14—H14C	0.96
O4—C23	1.235 (2)	C15—H15A	0.96
N1—C1	1.478 (2)	C15—H15B	0.96
N1—C4	1.494 (2)	C15—H15C	0.96
N2—C23	1.387 (3)	C16—H16A	0.96
N2—C22	1.391 (2)	C16—H16B	0.96
N2—C24	1.473 (2)	C16—H16C	0.96
C1—C2	1.528 (2)	C17—C18	1.402 (3)
C1—H1A	0.97	C17—C22	1.413 (2)
C1—H1B	0.97	C18—C19	1.375 (3)
C2—C5	1.524 (3)	C18—H18	0.93
C2—C3	1.540 (2)	C19—C20	1.395 (3)
C2—H2	0.98	C19—H19	0.93
C3—C7	1.505 (3)	C20—C21	1.374 (3)
C3—C4	1.532 (3)	C20—H20	0.93
C3—H3	0.98	C21—C22	1.397 (3)
C4—C25B	1.527 (7)	C21—H21	0.93
C4—C25A	1.559 (3)	C24—H24A	0.96
C4—H4	0.98	C24—H24B	0.96
C4—H4B	0.96	C24—H24C	0.96
C5—C15	1.515 (3)	C25A—C26A	1.512 (4)
C5—C16	1.525 (3)	C25A—H25A	0.97
C6—C7	1.353 (3)	C25A—H25B	0.97
C6—C17	1.440 (3)	C26A—H26A	0.96
C7—C23	1.455 (2)	C26A—H26B	0.96
C8—C13	1.389 (2)	C26A—H26C	0.96
C8—C9	1.398 (2)	C25B—C26B	1.503 (8)
C9—C10	1.385 (3)	C25B—H25C	0.97
C9—H9	0.93	C25B—H25D	0.97
C10—C11	1.392 (3)	C26B—H26D	0.96
C10—H10	0.93	C26B—H26E	0.96
C11—C12	1.393 (2)	C26B—H26F	0.96
C11—C14	1.505 (3)		
O2—S1—O1	119.40 (9)	C12—C13—H13	120.3

O2—S1—N1	106.87 (8)	C8—C13—H13	120.3
O1—S1—N1	106.65 (8)	C11—C14—H14A	109.5
O2—S1—C8	108.47 (8)	C11—C14—H14B	109.5
O1—S1—C8	106.76 (8)	H14A—C14—H14B	109.5
N1—S1—C8	108.29 (8)	C11—C14—H14C	109.5
C6—O3—C5	117.44 (14)	H14A—C14—H14C	109.5
C1—N1—C4	110.90 (14)	H14B—C14—H14C	109.5
C1—N1—S1	117.64 (12)	C5—C15—H15A	109.5
C4—N1—S1	121.48 (13)	C5—C15—H15B	109.5
C23—N2—C22	122.96 (15)	H15A—C15—H15B	109.5
C23—N2—C24	117.89 (16)	C5—C15—H15C	109.5
C22—N2—C24	119.06 (16)	H15A—C15—H15C	109.5
N1—C1—C2	104.28 (14)	H15B—C15—H15C	109.5
N1—C1—H1A	110.9	C5—C16—H16A	109.5
C2—C1—H1A	110.9	C5—C16—H16B	109.5
N1—C1—H1B	110.9	H16A—C16—H16B	109.5
C2—C1—H1B	110.9	C5—C16—H16C	109.5
H1A—C1—H1B	108.9	H16A—C16—H16C	109.5
C5—C2—C1	113.45 (16)	H16B—C16—H16C	109.5
C5—C2—C3	113.65 (16)	C18—C17—C22	119.19 (17)
C1—C2—C3	103.88 (14)	C18—C17—C6	122.58 (16)
C5—C2—H2	108.5	C22—C17—C6	118.21 (17)
C1—C2—H2	108.5	C19—C18—C17	121.08 (17)
C3—C2—H2	108.5	C19—C18—H18	119.5
C7—C3—C4	114.57 (16)	C17—C18—H18	119.5
C7—C3—C2	110.00 (16)	C18—C19—C20	119.16 (19)
C4—C3—C2	102.90 (15)	C18—C19—H19	120.4
C7—C3—H3	109.7	C20—C19—H19	120.4
C4—C3—H3	109.7	C21—C20—C19	121.09 (19)
C2—C3—H3	109.7	C21—C20—H20	119.5
N1—C4—C25B	112.8 (3)	C19—C20—H20	119.5
N1—C4—C3	103.94 (14)	C20—C21—C22	120.41 (17)
C25B—C4—C3	131.3 (3)	C20—C21—H21	119.8
N1—C4—C25A	109.35 (17)	C22—C21—H21	119.8
C3—C4—C25A	106.26 (18)	N2—C22—C21	121.58 (16)
N1—C4—H4	112.3	N2—C22—C17	119.35 (17)
C25B—C4—H4	82.6	C21—C22—C17	119.05 (17)
C3—C4—H4	112.3	O4—C23—N2	120.50 (17)
C25A—C4—H4	112.3	O4—C23—C7	122.04 (18)
N1—C4—H4B	101.6	N2—C23—C7	117.46 (17)
C25B—C4—H4B	101.3	N2—C24—H24A	109.5
C3—C4—H4B	101.5	N2—C24—H24B	109.5
C25A—C4—H4B	131.3	H24A—C24—H24B	109.5
O3—C5—C15	104.91 (16)	N2—C24—H24C	109.5
O3—C5—C2	109.40 (14)	H24A—C24—H24C	109.5
C15—C5—C2	111.60 (16)	H24B—C24—H24C	109.5
O3—C5—C16	107.99 (16)	C26A—C25A—C4	113.6 (2)
C15—C5—C16	111.17 (16)	C26A—C25A—H25A	108.8
C2—C5—C16	111.47 (17)	C4—C25A—H25A	108.8

C7—C6—O3	124.43 (17)	C26A—C25A—H25B	108.8
C7—C6—C17	121.63 (16)	C4—C25A—H25B	108.8
O3—C6—C17	113.94 (16)	H25A—C25A—H25B	107.7
C6—C7—C23	120.05 (17)	C25A—C26A—H26A	109.5
C6—C7—C3	122.30 (16)	C25A—C26A—H26B	109.5
C23—C7—C3	117.56 (17)	H26A—C26A—H26B	109.5
C13—C8—C9	120.55 (18)	C25A—C26A—H26C	109.5
C13—C8—S1	119.56 (13)	H26A—C26A—H26C	109.5
C9—C8—S1	119.86 (14)	H26B—C26A—H26C	109.5
C10—C9—C8	118.98 (17)	C26B—C25B—C4	105.4 (5)
C10—C9—H9	120.5	C26B—C25B—H25C	110.7
C8—C9—H9	120.5	C4—C25B—H25C	110.7
C9—C10—C11	121.35 (17)	C26B—C25B—H25D	110.7
C9—C10—H10	119.3	C4—C25B—H25D	110.7
C11—C10—H10	119.3	H25C—C25B—H25D	108.8
C10—C11—C12	118.55 (18)	C25B—C26B—H26D	109.5
C10—C11—C14	120.77 (17)	C25B—C26B—H26E	109.5
C12—C11—C14	120.68 (17)	H26D—C26B—H26E	109.5
C13—C12—C11	121.18 (17)	C25B—C26B—H26F	109.5
C13—C12—H12	119.4	H26D—C26B—H26F	109.5
C11—C12—H12	119.4	H26E—C26B—H26F	109.5
C12—C13—C8	119.38 (16)		
O2—S1—N1—C1	175.21 (13)	N1—S1—C8—C13	−95.57 (15)
O1—S1—N1—C1	−56.03 (15)	O2—S1—C8—C9	−33.33 (17)
C8—S1—N1—C1	58.53 (15)	O1—S1—C8—C9	−163.20 (14)
O2—S1—N1—C4	32.76 (16)	N1—S1—C8—C9	82.31 (16)
O1—S1—N1—C4	161.52 (14)	C13—C8—C9—C10	0.6 (3)
C8—S1—N1—C4	−83.92 (15)	S1—C8—C9—C10	−177.22 (14)
C4—N1—C1—C2	−10.4 (2)	C8—C9—C10—C11	−0.5 (3)
S1—N1—C1—C2	−156.59 (12)	C9—C10—C11—C12	−0.3 (3)
N1—C1—C2—C5	153.67 (15)	C9—C10—C11—C14	179.68 (18)
N1—C1—C2—C3	29.77 (19)	C10—C11—C12—C13	1.1 (3)
C5—C2—C3—C7	−39.1 (2)	C14—C11—C12—C13	−178.91 (17)
C1—C2—C3—C7	84.63 (18)	C11—C12—C13—C8	−1.0 (3)
C5—C2—C3—C4	−161.64 (15)	C9—C8—C13—C12	0.1 (3)
C1—C2—C3—C4	−37.87 (18)	S1—C8—C13—C12	177.97 (13)
C1—N1—C4—C25B	134.0 (4)	C7—C6—C17—C18	−178.76 (17)
S1—N1—C4—C25B	−81.3 (4)	O3—C6—C17—C18	1.9 (2)
C1—N1—C4—C3	−13.2 (2)	C7—C6—C17—C22	−0.3 (3)
S1—N1—C4—C3	131.45 (14)	O3—C6—C17—C22	−179.61 (15)
C1—N1—C4—C25A	99.89 (19)	C22—C17—C18—C19	1.1 (3)
S1—N1—C4—C25A	−115.41 (18)	C6—C17—C18—C19	179.58 (17)
C7—C3—C4—N1	−88.26 (18)	C17—C18—C19—C20	0.5 (3)
C2—C3—C4—N1	31.12 (18)	C18—C19—C20—C21	−1.3 (3)
C7—C3—C4—C25B	133.3 (4)	C19—C20—C21—C22	0.6 (3)
C2—C3—C4—C25B	−107.3 (4)	C23—N2—C22—C21	178.04 (16)
C7—C3—C4—C25A	156.40 (17)	C24—N2—C22—C21	1.6 (3)
C2—C3—C4—C25A	−84.23 (18)	C23—N2—C22—C17	0.0 (3)
C6—O3—C5—C15	−163.06 (15)	C24—N2—C22—C17	−176.48 (16)

C6—O3—C5—C2	−43.2 (2)	C20—C21—C22—N2	−177.01 (17)
C6—O3—C5—C16	78.29 (19)	C20—C21—C22—C17	1.1 (3)
C1—C2—C5—O3	−63.18 (19)	C18—C17—C22—N2	176.24 (16)
C3—C2—C5—O3	55.21 (19)	C6—C17—C22—N2	−2.3 (2)
C1—C2—C5—C15	52.5 (2)	C18—C17—C22—C21	−1.9 (3)
C3—C2—C5—C15	170.86 (16)	C6—C17—C22—C21	179.59 (16)
C1—C2—C5—C16	177.44 (16)	C22—N2—C23—O4	−175.84 (17)
C3—C2—C5—C16	−64.2 (2)	C24—N2—C23—O4	0.6 (3)
C5—O3—C6—C7	16.5 (2)	C22—N2—C23—C7	4.6 (2)
C5—O3—C6—C17	−164.19 (14)	C24—N2—C23—C7	−178.86 (15)
O3—C6—C7—C23	−175.72 (15)	C6—C7—C23—O4	173.38 (17)
C17—C6—C7—C23	5.0 (3)	C3—C7—C23—O4	−3.1 (3)
O3—C6—C7—C3	0.6 (3)	C6—C7—C23—N2	−7.1 (3)
C17—C6—C7—C3	−178.68 (16)	C3—C7—C23—N2	176.42 (15)
C4—C3—C7—C6	126.67 (18)	N1—C4—C25A—C26A	63.3 (3)
C2—C3—C7—C6	11.4 (2)	C25B—C4—C25A—C26A	−38.9 (6)
C4—C3—C7—C23	−56.9 (2)	C3—C4—C25A—C26A	174.9 (2)
C2—C3—C7—C23	−172.27 (15)	N1—C4—C25B—C26B	−65.5 (6)
O2—S1—C8—C13	148.80 (14)	C3—C4—C25B—C26B	70.1 (6)
O1—S1—C8—C13	18.93 (17)	C25A—C4—C25B—C26B	24.8 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O1^{i}	0.98	2.48	3.282 (2)	139
C4—H4···O4	0.98	2.38	2.974 (2)	118
C25A—H25A···Cg1^{ii}	0.97	2.87	3.706 (3)	145

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

Fig. 1

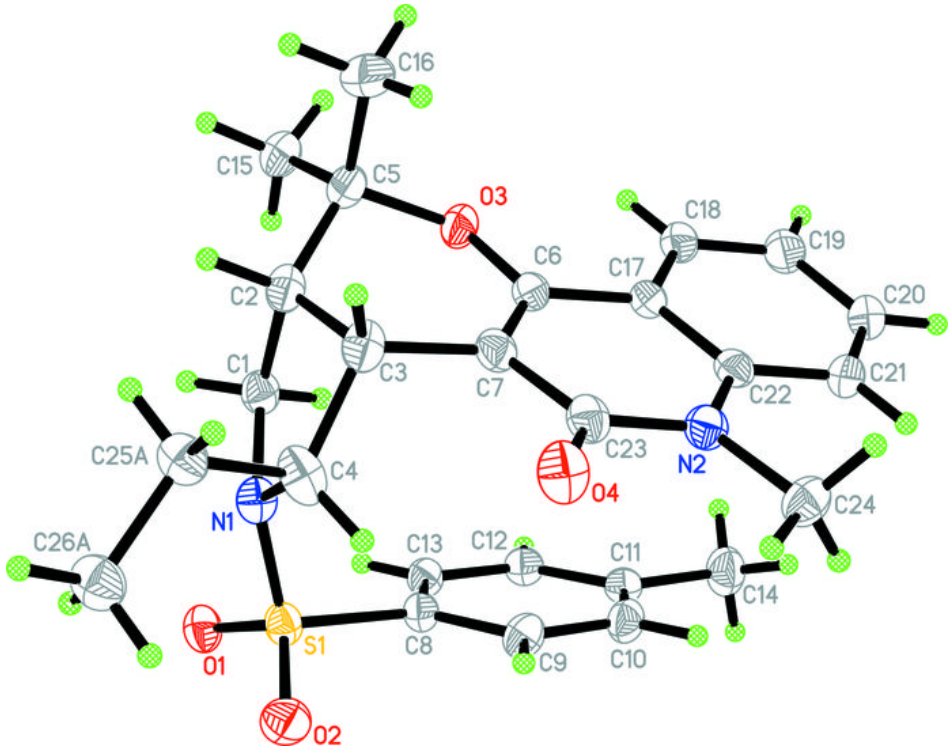
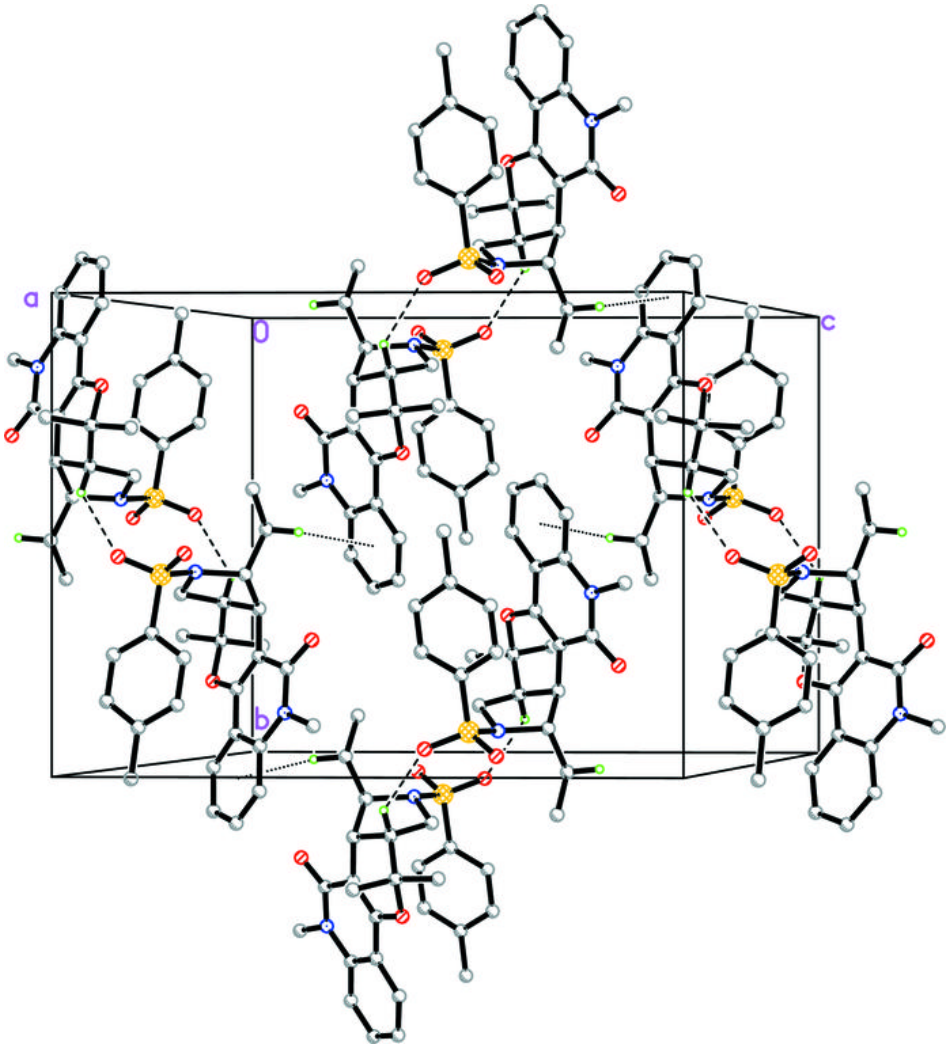

C16
C15
C5
O3
C18
C19
C6
C17
C20
C2
C1
C3
C7
C22
C21
C25A
C4
C23
N2
O4
N1
C24
C26A
C13
C12
C11
C14
O1
S1
C8
C9
C10
O2

Fig. 2



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Seven papers on fused-ring heterocyclic ketones containing an *N*-tosyl-pyrrolo[3,4-*c*]pyrano moiety. Corrigenda

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Corrections are made to the name of an author in seven papers by Chinnakali *et al.* [*Acta Cryst.* (2007), E**63**, o4363, o4364, o4434–o4435, o4436–o4437, o4438, o4489–o4490 and o4491–o4492].

In the papers by Chinnakali, Jayagopi *et al.* (2007*a*,*b*) and Chinnakali, Sudha *et al.* (2007*a*,*b*,*c*,*d*,*e*), the name of the author M. Jayagopi is given incorrectly. The correct name should be M. Jayagobi, as given above.

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