Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4,4-Dimethyl-2-tosyl-2,3,3a,4-tetrahydro-1*H*,10*H*-pyrrolo[3,4-*c*]pyrano[6,5-*b*]indan-10-one

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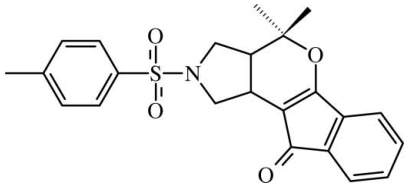
Received 19 October 2007; accepted 21 October 2007

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.001 Å; R factor = 0.034; wR factor = 0.105; data-to-parameter ratio = 32.8.

The molecule of the title compound, $C_{23}H_{23}NO_4S$, adopts a folded conformation, with the cyclopentadienone ring and tosyl groups arranged in an almost face-to-face fashion. The pyrrolidine ring has an envelope conformation and the dihydropyran ring is in a half-chair conformation. The pyrrolidine and dihydropyran rings are *cis*-fused. The indenone ring system is essentially planar, and the indene plane forms a dihedral angle of 25.12 (3)° with the sulfonyl-bound benzene ring. In the crystal structure, molecules translated by one unit cell along the *a*-axis direction are linked into a chain by C—H···O hydrogen bonds. The inversion-related molecules of adjacent chains are linked along the *c* axis by C—H···O hydrogen bonds into a sheet-like structure parallel to the *ac* plane.

Related literature

For bond-length data, see: Allen *et al.* (1987). For related pyrrolo[3,4-*c*]pyran structures, see: Chinnakali *et al.* (2007*a*,*b*). For ring-puckering parameters, see: Cremer & Pople (1975). For asymmetry parameters, see: Duax *et al.* (1976). For notation of hydrogen-bonding motifs, see: Bernstein *et al.* (1995).



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Experimental

Crystal data

$C_{23}H_{23}NO_4S$
M_r = 409.48
Triclinic, $P\overline{1}$
a = 8.0219 (2) Å
b = 8.6106 (2) Å
c = 15.0432 (4) Å
α = 104.557 (1)°
β = 99.182 (1)°
γ = 93.192 (1)°
V = 987.84 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.19 mm^{-1}
T = 100.0 (1) K
0.60 × 0.56 × 0.37 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.862, T_{max} = 0.932
42977 measured reflections
8635 independent reflections
7903 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.106
S = 1.07
8635 reflections
263 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O1^{i}	0.98	2.45	3.2451 (10)	138
C16—H16A···O3^{ii}	0.96	2.55	3.5075 (11)	175
C16—H16C···O1^{i}	0.96	2.49	3.4151 (11)	161
C21—H21···O4^{iii}	0.93	2.56	3.2266 (9)	129

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

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).

HKF thanks Universiti Sains Malaysia for Fundamental Research Grant Scheme (FRGS) grant No. 203/PFIZIK/671064.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2211).

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  doi:10.1107/S1600536807052233

supplementary materials

Acta Cryst. (2007). E**63**, o4438 [**doi:10.1107/S1600536807052233**]

4,4-Dimethyl-2-tosyl-2,3,3a,4-tetrahydro-1*H*,10*H*-pyrrolo[3,4-*c*]pyrano[6,5-*b*]indan-10-one

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

Comment

As part of our ongoing studies on pyrrolo[3,4-*c*]pyran derivatives (Chinnakali *et al.*, 2007*a*,b), we report here the crystal structure of the title compound (Fig. 1).

Bond lengths and angles show normal values (Allen *et al.*, 1987), and are comparable with those in related structures (Chinnakali *et al.*, 2007*a*,b). As a result of the repulsive interaction between the short S═O bonds, atom S1 has a distorted tetrahedral configuration, with the O2—S1—O1 [120.17 (4)°] angle deviating significantly from the ideal tetrahedral value.

The pyrrolidine ring (N1/C1–C4) has an envelope conformation with atom C2 deviating by 0.586 (1) Å from the least-squares plane formed by the remaining four ring atoms. The puckering parameters (q_2, φ_2; Cremer & Pople, 1975) and the smallest displacement asymmetry parameters (Duax *et al.*, 1976) for the pyrrolidine ring are q_2 = 0.3821 (8) Å, φ_2 = 260.23 (11)° and ΔC_s[C2] = 6.18 (7)°. The tosyl group is equatorially attached to the pyrrolidine ring. The dihydropyran ring adopts a half-chair conformation with a local twofold rotation axis passing through the C2—C5 and C6—C7 bonds; the puckering (Q, θ, φ) and asymmetry (ΔC_2[C2–C5]) parameters are 0.4439 (8) Å, 129.98 (10)°, 276.03 (12)° and 3.45 (9)°, respectively. The pyrrolidine and dihydropyran rings are *cis*-fused.

The indenone ring system is essentially planar, with atom O4 deviating from the indene plane by 0.088 (1) Å. The dihedral angle between the indene ring system and the C8–C13 benzene ring is 25.12 (3)°. The molecule adopts a folded conformation, with the cyclopentadienone and C8–C13 benzene rings arranged in an almost face-to-face fashion. However, no significant π–π interactions are observed between these rings as their centroids are separated by 3.9135 (5) Å.

In the crystal structure, molecules translated by one unit cell along the *a*-axis direction are linked by C3—H3···O1^{i} and C16—H16C···O1^{i} [symmetry code: (i) 1 + *x*, *y*, *z*] hydrogen-bonding interactions to form a chain. These interactions together constitute a pair of bifurcated acceptor bonds, generating an $R^1_2(7)$ motif (Bernstein *et al.*, 1995). The inversion-related molecules of adjacent chains are alternately linked along the *c* axis by pairs of C16—H16A···O3^{ii} and C21—H21···O4^{iii} [symmetry codes: (ii) 2 − *x*, 2 − *y*, −*z*; (iii) 2 − *x*, 2 − *y*, 1 − *z*] hydrogen bonds (Table 1) into a sheet-like structure parallel to the *ac* plane (Fig. 2). The pairs of C16—H16A···O3^{ii} and C21—H21···O4^{iii} interactions generate rings of graph-set motif $R^2_2(10)$ and $R^2_2(8)$, respectively.

Experimental

To a solution of 2*H*-indene-1,3-dione (1 mmol) in dry toluene (20 ml), 2-[*N*-(3-methylbut-2-enyl)-*N*-tosylamino]acetaldehyde (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

H atoms were positioned geometrically (C—H = 0.93–0.98 Å) and allowed to ride on their parent atoms, with U_{iso}(H) = 1.5U_{eq}(C_{methyl}) or 1.2U_{eq}(C). A rotating group model was used for the methyl group attached to the aromatic ring.

Figures

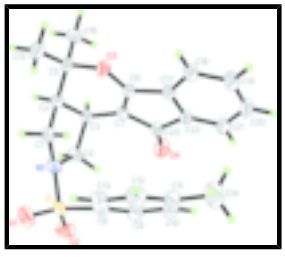


Fig. 1. The molecular structure of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 80% probability level.

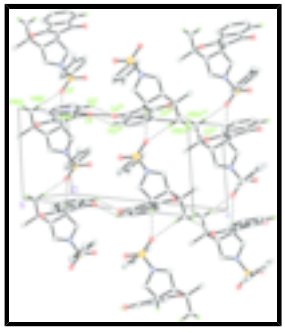


Fig. 2. View of a hydrogen-bonded (dashed lines) sheet of the title compound. For the sake of clarity, H atoms not involved in the interactions have been omitted. Symmetry codes: (i) 1 + *x*, *y*, *z*; (iii) 2 − *x*, 2 − *y*, 1 − *z*; (iv) *x*, *y*, 1 + *z*.

4,4-Dimethyl-2-tosyl-2,3,3a,4-tetrahydro-1H,10*H*- pyrrolo[3,4-*c*]pyrano[6,5-*b*]indan-10-one

Crystal data

$C_{23}H_{23}NO_4S$	Z = 2
M_r = 409.48	F_{000} = 432
Triclinic, $P\overline{1}$	D_x = 1.377 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 8.0219 (2) Å	Cell parameters from 8302 reflections
b = 8.6106 (2) Å	θ = 2.5–40.2º
c = 15.0432 (4) Å	μ = 0.19 mm^{-1}
α = 104.557 (1)º	T = 100.0 (1) K
β = 99.182 (1)º	Block, light yellow
γ = 93.192 (1)º	0.60 × 0.56 × 0.37 mm
V = 987.84 (4) Å^3	

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	8635 independent reflections

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} = 0.862, T_{max} = 0.932
42977 measured reflections
7903 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 35.0º
θ_{min} = 1.4º
h = −12→12
k = −13→13
l = −24→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.106
S = 1.07
8635 reflections
263 parameters
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
$w = 1/[\sigma^2(F_o^2) + (0.0596P)^2 + 0.2351P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 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}
S1	0.39580 (2)	0.63360 (2)	0.220153 (13)	0.01541 (5)
O1	0.23678 (8)	0.62916 (8)	0.15941 (5)	0.02275 (12)
O2	0.41576 (9)	0.52386 (7)	0.27782 (5)	0.02174 (12)
O3	0.83313 (8)	0.95635 (6)	0.09401 (4)	0.01588 (10)
O4	0.99483 (9)	0.77446 (7)	0.36449 (4)	0.02030 (11)
N1	0.53669 (8)	0.59825 (7)	0.15218 (4)	0.01406 (10)
C1	0.55116 (9)	0.69996 (9)	0.08746 (5)	0.01553 (12)

H1A	0.5482	0.8129	0.1182	0.019*
H1B	0.4608	0.6678	0.0334	0.019*
C2	0.72446 (9)	0.66848 (8)	0.05984 (5)	0.01418 (11)
H2	0.7114	0.5658	0.0118	0.017*
C3	0.83158 (9)	0.64700 (8)	0.15018 (5)	0.01296 (11)
H3	0.9272	0.5848	0.1361	0.016*
C4	0.70506 (9)	0.55341 (8)	0.18884 (5)	0.01496 (11)
H4A	0.7108	0.4381	0.1671	0.018*
H4B	0.7277	0.5847	0.2566	0.018*
C5	0.80278 (10)	0.79956 (8)	0.02205 (5)	0.01600 (12)
C6	0.88902 (9)	0.94690 (8)	0.18073 (5)	0.01282 (11)
C7	0.89279 (9)	0.81174 (8)	0.21169 (5)	0.01246 (11)
C8	0.44908 (9)	0.83213 (9)	0.29019 (5)	0.01570 (12)
C9	0.56938 (10)	0.86295 (10)	0.37214 (5)	0.01873 (13)
H9	0.6141	0.7784	0.3930	0.022*
C10	0.62124 (11)	1.02188 (10)	0.42204 (6)	0.02109 (14)
H10	0.7008	1.0433	0.4769	0.025*
C11	0.55587 (11)	1.15034 (10)	0.39124 (6)	0.02036 (14)
C12	0.43419 (11)	1.11695 (10)	0.30990 (6)	0.02146 (14)
H12	0.3886	1.2014	0.2893	0.026*
C13	0.38025 (10)	0.95850 (10)	0.25916 (6)	0.01916 (13)
H13	0.2989	0.9370	0.2050	0.023*
C14	0.61644 (14)	1.32121 (11)	0.44569 (8)	0.0315 (2)
H14A	0.5504	1.3937	0.4193	0.047*
H14B	0.7338	1.3436	0.4430	0.047*
H14C	0.6038	1.3354	0.5095	0.047*
C15	0.68402 (13)	0.83273 (10)	−0.05901 (6)	0.02343 (16)
H15A	0.7383	0.9153	−0.0803	0.035*
H15B	0.5815	0.8679	−0.0388	0.035*
H15C	0.6573	0.7359	−0.1091	0.035*
C16	0.97315 (11)	0.75615 (10)	−0.00403 (6)	0.02156 (15)
H16A	1.0209	0.8391	−0.0276	0.032*
H16B	0.9573	0.6554	−0.0512	0.032*
H16C	1.0488	0.7466	0.0502	0.032*
C17	0.95601 (9)	1.09335 (8)	0.25648 (5)	0.01349 (11)
C18	0.97941 (10)	1.25424 (9)	0.25762 (5)	0.01705 (12)
H18	0.9517	1.2876	0.2034	0.020*
C19	1.04670 (11)	1.36602 (9)	0.34373 (6)	0.02031 (14)
H19	1.0648	1.4749	0.3465	0.024*
C20	1.08615 (11)	1.31523 (10)	0.42432 (6)	0.02093 (14)
H20	1.1278	1.3910	0.4808	0.025*
C21	1.06429 (10)	1.15118 (9)	0.42228 (5)	0.01811 (13)
H21	1.0919	1.1172	0.4763	0.022*
C22	1.00078 (9)	1.04233 (8)	0.33774 (5)	0.01415 (11)
C23	0.96614 (9)	0.86138 (8)	0.31201 (5)	0.01398 (11)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.01277 (8)	0.01370 (8)	0.01945 (8)	−0.00091 (5)	0.00437 (6)	0.00339 (6)
O1	0.0122 (2)	0.0237 (3)	0.0283 (3)	−0.0010 (2)	0.0010 (2)	0.0016 (2)
O2	0.0258 (3)	0.0168 (2)	0.0261 (3)	0.0000 (2)	0.0109 (2)	0.0087 (2)
O3	0.0234 (3)	0.0116 (2)	0.0113 (2)	−0.00181 (18)	0.00137 (17)	0.00251 (16)
O4	0.0277 (3)	0.0166 (2)	0.0169 (2)	0.0031 (2)	0.0006 (2)	0.00693 (19)
N1	0.0124 (2)	0.0139 (2)	0.0163 (2)	0.00059 (18)	0.00296 (18)	0.00469 (19)
C1	0.0147 (3)	0.0155 (3)	0.0161 (3)	−0.0007 (2)	0.0002 (2)	0.0056 (2)
C2	0.0165 (3)	0.0118 (3)	0.0131 (3)	−0.0018 (2)	0.0026 (2)	0.0020 (2)
C3	0.0131 (3)	0.0104 (2)	0.0150 (3)	0.00002 (19)	0.0033 (2)	0.00229 (19)
C4	0.0133 (3)	0.0129 (3)	0.0198 (3)	0.0007 (2)	0.0031 (2)	0.0065 (2)
C5	0.0226 (3)	0.0125 (3)	0.0115 (3)	−0.0027 (2)	0.0032 (2)	0.0013 (2)
C6	0.0145 (3)	0.0111 (2)	0.0121 (2)	−0.0003 (2)	0.0023 (2)	0.00204 (19)
C7	0.0133 (3)	0.0106 (2)	0.0129 (3)	0.00010 (19)	0.0021 (2)	0.00233 (19)
C8	0.0144 (3)	0.0150 (3)	0.0176 (3)	0.0017 (2)	0.0040 (2)	0.0034 (2)
C9	0.0201 (3)	0.0172 (3)	0.0182 (3)	0.0039 (2)	0.0030 (2)	0.0033 (2)
C10	0.0208 (3)	0.0194 (3)	0.0199 (3)	0.0032 (3)	0.0021 (3)	0.0000 (2)
C11	0.0198 (3)	0.0160 (3)	0.0237 (3)	0.0021 (2)	0.0071 (3)	0.0001 (2)
C12	0.0225 (3)	0.0159 (3)	0.0265 (4)	0.0051 (3)	0.0059 (3)	0.0050 (3)
C13	0.0177 (3)	0.0171 (3)	0.0221 (3)	0.0040 (2)	0.0023 (2)	0.0045 (2)
C14	0.0332 (5)	0.0175 (4)	0.0372 (5)	0.0005 (3)	0.0063 (4)	−0.0044 (3)
C15	0.0344 (4)	0.0192 (3)	0.0143 (3)	−0.0040 (3)	−0.0016 (3)	0.0051 (2)
C16	0.0268 (4)	0.0185 (3)	0.0202 (3)	−0.0023 (3)	0.0116 (3)	0.0030 (2)
C17	0.0154 (3)	0.0106 (2)	0.0135 (3)	0.0005 (2)	0.0023 (2)	0.00183 (19)
C18	0.0216 (3)	0.0115 (3)	0.0172 (3)	0.0007 (2)	0.0032 (2)	0.0028 (2)
C19	0.0257 (4)	0.0115 (3)	0.0210 (3)	−0.0008 (2)	0.0032 (3)	0.0006 (2)
C20	0.0256 (4)	0.0147 (3)	0.0178 (3)	−0.0013 (3)	0.0010 (3)	−0.0018 (2)
C21	0.0212 (3)	0.0162 (3)	0.0139 (3)	−0.0002 (2)	0.0001 (2)	0.0008 (2)
C22	0.0155 (3)	0.0123 (3)	0.0134 (3)	0.0005 (2)	0.0015 (2)	0.0019 (2)
C23	0.0148 (3)	0.0126 (3)	0.0139 (3)	0.0011 (2)	0.0019 (2)	0.0029 (2)

Geometric parameters (Å, °)

S1—O2	1.4337 (6)	C9—H9	0.93
S1—O1	1.4383 (7)	C10—C11	1.3992 (12)
S1—N1	1.6329 (6)	C10—H10	0.93
S1—C8	1.7563 (8)	C11—C12	1.3942 (13)
O3—C6	1.3343 (8)	C11—C14	1.5031 (12)
O3—C5	1.4827 (9)	C12—C13	1.3916 (12)
O4—C23	1.2226 (9)	C12—H12	0.93
N1—C1	1.4770 (9)	C13—H13	0.93
N1—C4	1.4849 (9)	C14—H14A	0.96
C1—C2	1.5325 (10)	C14—H14B	0.96
C1—H1A	0.97	C14—H14C	0.96
C1—H1B	0.97	C15—H15A	0.96
C2—C5	1.5328 (10)	C15—H15B	0.96

C2—C3	1.5462 (10)	C15—H15C	0.96
C2—H2	0.98	C16—H16A	0.96
C3—C7	1.4923 (9)	C16—H16B	0.96
C3—C4	1.5332 (10)	C16—H16C	0.96
C3—H3	0.98	C17—C18	1.3831 (10)
C4—H4A	0.97	C17—C22	1.4012 (10)
C4—H4B	0.97	C18—C19	1.4099 (11)
C5—C15	1.5202 (11)	C18—H18	0.93
C5—C16	1.5217 (12)	C19—C20	1.3859 (12)
C6—C7	1.3581 (9)	C19—H19	0.93
C6—C17	1.4779 (9)	C20—C21	1.4057 (11)
C7—C23	1.4734 (10)	C20—H20	0.93
C8—C13	1.3953 (11)	C21—C22	1.3770 (10)
C8—C9	1.3960 (11)	C21—H21	0.93
C9—C10	1.3892 (11)	C22—C23	1.5063 (10)
O2—S1—O1	120.17 (4)	C9—C10—C11	121.18 (8)
O2—S1—N1	106.46 (4)	C9—C10—H10	119.4
O1—S1—N1	105.76 (4)	C11—C10—H10	119.4
O2—S1—C8	109.35 (4)	C12—C11—C10	118.97 (7)
O1—S1—C8	107.78 (4)	C12—C11—C14	120.94 (8)
N1—S1—C8	106.52 (3)	C10—C11—C14	120.09 (8)
C6—O3—C5	114.81 (6)	C13—C12—C11	120.66 (8)
C1—N1—C4	111.34 (6)	C13—C12—H12	119.7
C1—N1—S1	118.53 (5)	C11—C12—H12	119.7
C4—N1—S1	119.42 (5)	C12—C13—C8	119.49 (7)
N1—C1—C2	103.05 (6)	C12—C13—H13	120.3
N1—C1—H1A	111.2	C8—C13—H13	120.3
C2—C1—H1A	111.2	C11—C14—H14A	109.5
N1—C1—H1B	111.2	C11—C14—H14B	109.5
C2—C1—H1B	111.2	H14A—C14—H14B	109.5
H1A—C1—H1B	109.1	C11—C14—H14C	109.5
C1—C2—C5	114.46 (6)	H14A—C14—H14C	109.5
C1—C2—C3	103.08 (5)	H14B—C14—H14C	109.5
C5—C2—C3	113.88 (6)	C5—C15—H15A	109.5
C1—C2—H2	108.4	C5—C15—H15B	109.5
C5—C2—H2	108.4	H15A—C15—H15B	109.5
C3—C2—H2	108.4	C5—C15—H15C	109.5
C7—C3—C4	113.62 (6)	H15A—C15—H15C	109.5
C7—C3—C2	107.12 (5)	H15B—C15—H15C	109.5
C4—C3—C2	103.12 (6)	C5—C16—H16A	109.5
C7—C3—H3	110.9	C5—C16—H16B	109.5
C4—C3—H3	110.9	H16A—C16—H16B	109.5
C2—C3—H3	110.9	C5—C16—H16C	109.5
N1—C4—C3	104.45 (6)	H16A—C16—H16C	109.5
N1—C4—H4A	110.9	H16B—C16—H16C	109.5
C3—C4—H4A	110.9	C18—C17—C22	121.23 (6)
N1—C4—H4B	110.9	C18—C17—C6	132.27 (7)
C3—C4—H4B	110.9	C22—C17—C6	106.50 (6)
H4A—C4—H4B	108.9	C17—C18—C19	117.81 (7)

O3—C5—C15	104.14 (6)	C17—C18—H18	121.1
O3—C5—C16	107.55 (6)	C19—C18—H18	121.1
C15—C5—C16	111.62 (7)	C20—C19—C18	120.64 (7)
O3—C5—C2	110.56 (5)	C20—C19—H19	119.7
C15—C5—C2	112.44 (6)	C18—C19—H19	119.7
C16—C5—C2	110.27 (6)	C19—C20—C21	121.16 (7)
O3—C6—C7	127.24 (6)	C19—C20—H20	119.4
O3—C6—C17	120.89 (6)	C21—C20—H20	119.4
C7—C6—C17	111.87 (6)	C22—C21—C20	117.92 (7)
C6—C7—C23	107.48 (6)	C22—C21—H21	121.0
C6—C7—C3	123.28 (6)	C20—C21—H21	121.0
C23—C7—C3	129.24 (6)	C21—C22—C17	121.20 (7)
C13—C8—C9	120.73 (7)	C21—C22—C23	130.91 (7)
C13—C8—S1	119.21 (6)	C17—C22—C23	107.89 (6)
C9—C8—S1	119.85 (6)	O4—C23—C7	127.46 (6)
C10—C9—C8	118.95 (7)	O4—C23—C22	126.32 (7)
C10—C9—H9	120.5	C7—C23—C22	106.23 (6)
C8—C9—H9	120.5		
O2—S1—N1—C1	−177.15 (5)	O1—S1—C8—C13	−23.07 (7)
O1—S1—N1—C1	53.96 (6)	N1—S1—C8—C13	90.05 (7)
C8—S1—N1—C1	−60.54 (6)	O2—S1—C8—C9	29.79 (7)
O2—S1—N1—C4	−35.69 (6)	O1—S1—C8—C9	162.01 (6)
O1—S1—N1—C4	−164.58 (5)	N1—S1—C8—C9	−84.87 (7)
C8—S1—N1—C4	80.92 (6)	C13—C8—C9—C10	−0.70 (12)
C4—N1—C1—C2	18.78 (7)	S1—C8—C9—C10	174.14 (6)
S1—N1—C1—C2	163.14 (5)	C8—C9—C10—C11	−0.40 (12)
N1—C1—C2—C5	−159.04 (6)	C9—C10—C11—C12	1.24 (13)
N1—C1—C2—C3	−34.83 (6)	C9—C10—C11—C14	−178.93 (8)
C1—C2—C3—C7	−81.83 (6)	C10—C11—C12—C13	−0.99 (13)
C5—C2—C3—C7	42.77 (8)	C14—C11—C12—C13	179.17 (8)
C1—C2—C3—C4	38.33 (6)	C11—C12—C13—C8	−0.07 (13)
C5—C2—C3—C4	162.92 (6)	C9—C8—C13—C12	0.93 (12)
C1—N1—C4—C3	5.19 (7)	S1—C8—C13—C12	−173.94 (6)
S1—N1—C4—C3	−138.82 (5)	O3—C6—C17—C18	−1.65 (12)
C7—C3—C4—N1	88.79 (7)	C7—C6—C17—C18	178.60 (8)
C2—C3—C4—N1	−26.79 (7)	O3—C6—C17—C22	179.12 (6)
C6—O3—C5—C15	160.01 (6)	C7—C6—C17—C22	−0.63 (8)
C6—O3—C5—C16	−81.43 (7)	C22—C17—C18—C19	−1.27 (11)
C6—O3—C5—C2	39.02 (9)	C6—C17—C18—C19	179.59 (8)
C1—C2—C5—O3	61.71 (8)	C17—C18—C19—C20	−0.60 (12)
C3—C2—C5—O3	−56.54 (8)	C18—C19—C20—C21	1.57 (13)
C1—C2—C5—C15	−54.22 (8)	C19—C20—C21—C22	−0.63 (13)
C3—C2—C5—C15	−172.46 (6)	C20—C21—C22—C17	−1.25 (12)
C1—C2—C5—C16	−179.49 (6)	C20—C21—C22—C23	178.69 (8)
C3—C2—C5—C16	62.27 (8)	C18—C17—C22—C21	2.25 (11)
C5—O3—C6—C7	−12.17 (10)	C6—C17—C22—C21	−178.42 (7)
C5—O3—C6—C17	168.12 (6)	C18—C17—C22—C23	−177.71 (7)
O3—C6—C7—C23	179.60 (7)	C6—C17—C22—C23	1.63 (8)
C17—C6—C7—C23	−0.67 (8)	C6—C7—C23—O4	−177.94 (8)

O3—C6—C7—C3	−0.19 (11)	C3—C7—C23—O4	1.83 (12)
C17—C6—C7—C3	179.54 (6)	C6—C7—C23—C22	1.63 (8)
C4—C3—C7—C6	−128.50 (7)	C3—C7—C23—C22	−178.61 (7)
C2—C3—C7—C6	−15.31 (9)	C21—C22—C23—O4	−2.41 (13)
C4—C3—C7—C23	51.76 (10)	C17—C22—C23—O4	177.54 (7)
C2—C3—C7—C23	164.96 (7)	C21—C22—C23—C7	178.01 (8)
O2—S1—C8—C13	−155.29 (6)	C17—C22—C23—C7	−2.03 (8)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O1^{i}	0.98	2.45	3.2451 (10)	138
C16—H16A···O3^{ii}	0.96	2.55	3.5075 (11)	175
C16—H16C···O1^{i}	0.96	2.49	3.4151 (11)	161
C21—H21···O4^{iii}	0.93	2.56	3.2266 (9)	129

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

Fig. 1

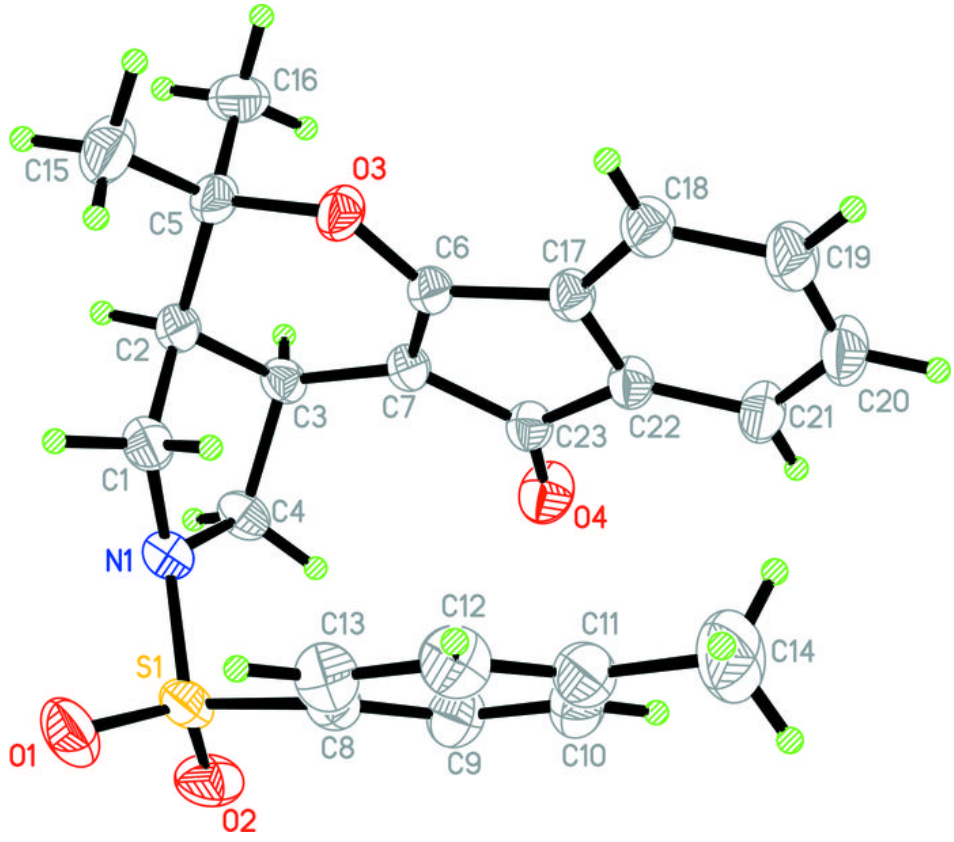
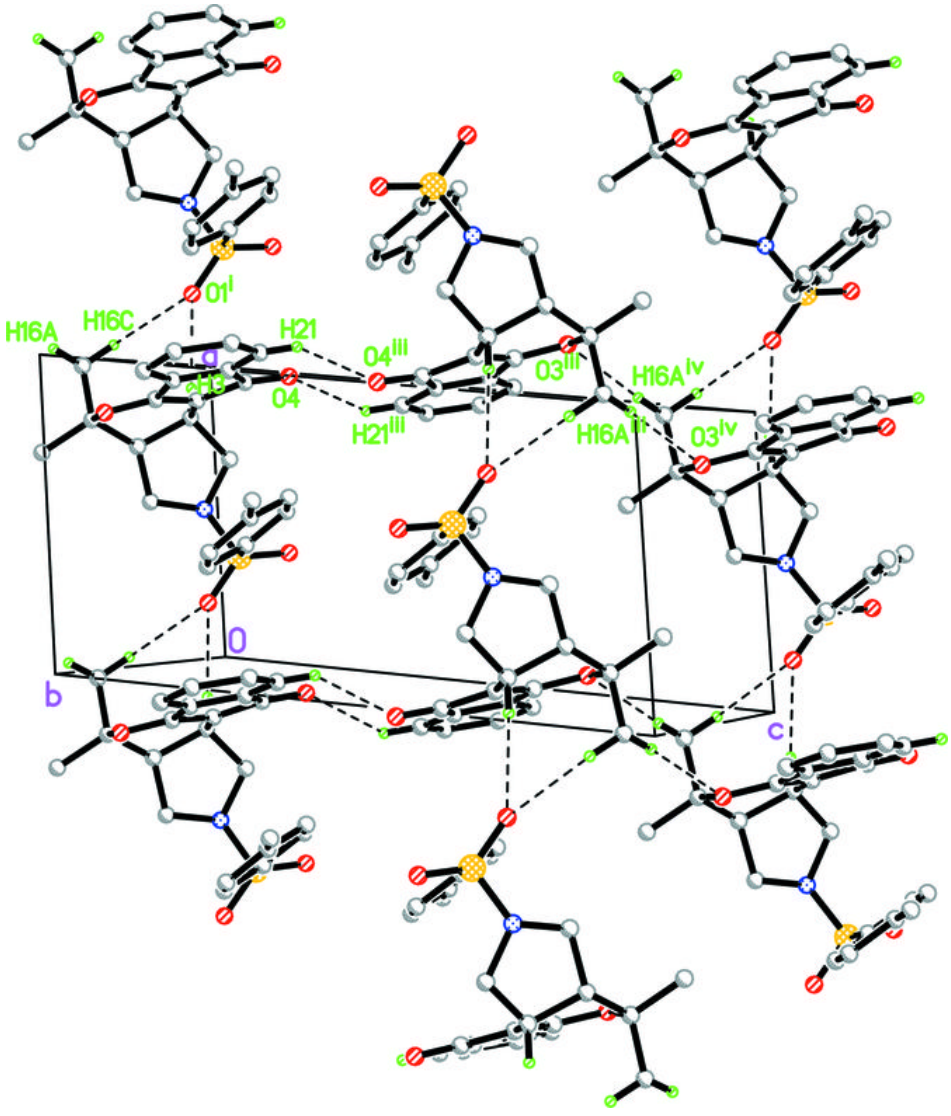

C16
C15
O3
C5
C18
C6
C17
C19
C2
C3
C7
C23
C22
C21
C20
C1
C4
O4
N1
C13
C12
C11
C14
S1
O1
C8
C9
C10
O2

Fig. 2


O1^{I}
H16A
H16C
H21
O4^{III}
O3^{III}
H16A^{IV}
H3
O4
H21^{III}
H16A^{III}
O3^{IV}
O
b
c

Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

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Received 26 November 2007; accepted 27 November 2007

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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 doi:10.1107/S1600536807063817