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4,4,6,8-Tetramethyl-2-tosylpyrrolo[3,4-*c*]-pyrano[6,5-*b*]pyrimidine-7,9-dione

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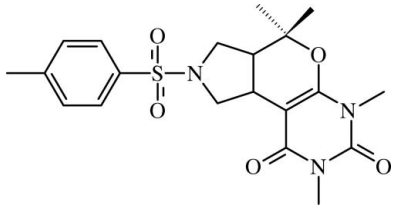
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.042; wR factor = 0.128; data-to-parameter ratio = 26.6.

In the title compound, $C_{20}H_{25}N_3O_5S$, the pyrrolidine ring is *trans*-fused to the dihydropyran ring. The pyrrolidine ring adopts a twist conformation and the dihydropyran ring is in an envelope conformation. The tosyl group is attached to the pyrrolidine ring in a biaxial position and its benzene ring forms a dihedral angle of 85.61 (4)° with the pyrimidine ring. The crystal packing shows that the molecules are linked into a three-dimensional framework through C—H···O hydrogen bonds.

Related literature

For biological activities of pyranopyrimidine derivatives, see: Abdel Fattah *et al.* (2004); Bedair *et al.* (2000, 2001); Eid *et al.* (2004); Shamroukh *et al.* (2007). For ring puckering parameters, see: Cremer & Pople (1975). For asymmetry parameters, see: Duax *et al.* (1976). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{20}H_{25}N_3O_5S$
M_r = 419.49
Monoclinic, $P2_1/c$
a = 14.5605 (2) Å
b = 8.9142 (1) Å
c = 15.3963 (3) Å
β = 94.316 (1)°
V = 1992.70 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.20 mm^{-1}
T = 100.0 (1) K
0.50 × 0.30 × 0.22 mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.906, T_{max} = 0.958
26688 measured reflections
7053 independent reflections
5564 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.128
S = 1.10
7053 reflections
265 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C15—H15A···O4^{i}	0.96	2.57	3.4571 (17)	153
C20—H20C···O5^{ii}	0.96	2.47	3.4125 (18)	168
C19—H19B···O2^{iii}	0.96	2.44	3.1917 (17)	134
C14—H14B···O1^{iv}	0.96	2.52	3.3787 (17)	149

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

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: IS2221).

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supplementary materials

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4,4,6,8-Tetramethyl-2-tosylpyrrolo[3,4-*c*]pyrano[6,5-*b*]pyrimidine-7,9-dione

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

Comment

Pyranopyrimidine derivatives exhibit antiviral (Shamroukh *et al.*, 2007) and antimicrobial activities (Bedair *et al.*, 2000, 2001; Eid *et al.*, 2004; Abdel Fattah *et al.*, 2004). We report here the crystal structure of the title compound, a pyranopyrimidine derivative.

In the molecule of the title compound (Fig. 1), bond lengths are within normal ranges (Allen *et al.*, 1987). The sum of the angles at the atom N1 of the pyrrolidine ring (347.9°) is in accordance with sp^3 hybridization. Atom S1 has a distorted tetrahedral configuration, with the angle O2—S1—O1 [120.33 (6)°] deviating significantly from the ideal tetrahedral value.

The pyrimidine ring is planar, with an r.m.s. deviation of fitted atoms of 0.009 Å, and atoms O4, O5, C19 and C20 deviating by 0.040 (2), 0.012 (2), 0.051 (2) and −0.011 (2) Å, respectively. The pyrrolidine ring adopts a twist conformation, confirmed by its ring-puckering parameters (Cremer & Pople, 1975) q_2 = 0.443 (1) Å and φ_2 = 92.3 (2)°, and asymmetry parameter (Duax *et al.*, 1976) ΔC_2[C2—C3] = 2.9 (1)°. The pyran ring adopts an envelope conformation, with atom C2 deviating from the C5/O3/C6/C7/C3 plane by 0.684 (2) Å. The asymmetry parameter ΔC_s[C2] is 3.8 (1)°, and the puckering parameters Q, θ and φ are 0.502 (1) Å, 129.5 (1)° and 295.3 (2)°, respectively. The tosyl group is attached to the pyrrolidine in a biaxial position and its benzene ring forms a dihedral angle of 85.61 (4)° with the pyrimidine ring. The dihedral angle between the C5/O3/C6/C7/C3 plane and the pyrimidine ring is 2.70 (8)°. The pyrrolidine ring is *trans*-fused to the dihydropyran ring.

In the crystal structure, inversion-related molecules are alternately linked by a pair each of C15—H15A···O4^{i} and C20—H20C···O5^{ii} hydrogen bonds to form a chain along the *b* axis (Fig. 2). Glide-related molecules in the adjacent chains are linked *via* C19—H19B···O2^{iii} hydrogen bonds, forming a two-dimensional network parallel to the *bc* plane. Screw-related molecules in the adjacent networks are cross-linked by C14—H14B···O1^{iv} hydrogen bonds (symmetry codes are given in Table 1) into a three-dimensional framework (Fig. 3).

Experimental

To a solution of 1,3-dimethyl pyrimidine-2,4,6-trione (1 mmol) in dry toluene (20 ml), the corresponding 2-[*N*-(3-methylbut-2-enyl)-*N*-tosylamino] acetaldehyde (1 mmol), and catalytic amount of the base ethylenediamine-*N*,*N*'-diacetate (EDDA) were added and the reaction mixture was refluxed for 12 h. After completion of 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) = 1.2U_{eq}(C) or 1.5U_{eq}(C_{methyl}). A rotating group model was used for the methyl groups attached to aromatic rings.

Figures

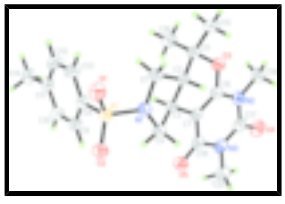


Fig. 1. The molecular structure of the title compound, showing 80% probability displacement ellipsoids and the atomic numbering.

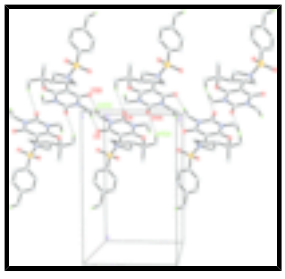


Fig. 2. View of a hydrogen-bonded (dashed lines) chain in the title compound. Atoms labelled with the suffixes A and B are generated by the symmetry operations (−*x*, 1 − *y*, 1 − *z*) and (−*x*, −*y*, 1 − *z*), respectively. For the sake of clarity, H atoms not involved in the interactions have been omitted.

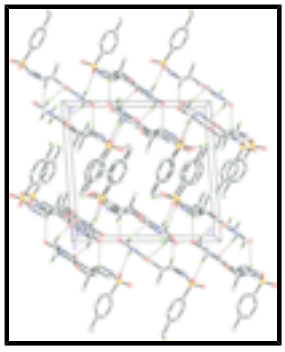


Fig. 3. The crystal packing of the title compound, viewed along the *b* axis. Hydrogen bonds are shown as dashed lines. For the sake of clarity, H atoms not involved in the interactions have been omitted.

4,4,6,8-Tetramethyl-2-tosylpyrrolo[3,4-*c*]pyrano[6,5-*b*]pyrimidine- 7,9-dione

Crystal data

$C_{20}H_{25}N_3O_5S$	F_{000} = 888
M_r = 419.49	D_x = 1.398 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 7931 reflections
a = 14.5605 (2) Å	θ = 2.6–34.9º
b = 8.9142 (1) Å	μ = 0.20 mm^{-1}
c = 15.3963 (3) Å	*T* = 100.0 (1) K
β = 94.316 (1)º	Block, light-yellow
V = 1992.70 (5) Å^3	0.50 × 0.30 × 0.22 mm

$Z = 4$

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer	7053 independent reflections
Radiation source: fine-focus sealed tube	5564 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.036$
Detector resolution: 8.33 pixels mm^{-1}	$\theta_{max} = 32.5°$
$T = 100.0(1)$ K	$\theta_{min} = 1.4°$
ω scans	$h = -21 \rightarrow 21$
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)	$k = -13 \rightarrow 13$
$T_{min} = 0.906$, $T_{max} = 0.958$	$l = -21 \rightarrow 23$
26688 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.042$	H-atom parameters constrained
$wR(F^2) = 0.128$	$w = 1/[\sigma^2(F_o^2) + (0.0646P)^2 + 0.4491P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.10$	$(\Delta/\sigma)_{max} = 0.001$
7053 reflections	$\Delta\rho_{max} = 0.48$ e Å^{-3}
265 parameters	$\Delta\rho_{min} = -0.37$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	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	0.31057 (2)	0.11286 (3)	0.21463 (2)	0.01524 (8)
O1	0.33383 (6)	0.19239 (11)	0.13827 (6)	0.02021 (19)

O2	0.27045 (6)	−0.03417 (10)	0.20717 (7)	0.01941 (19)
O3	0.17594 (6)	0.57429 (10)	0.47387 (7)	0.01950 (19)
O4	0.00954 (7)	0.39530 (12)	0.68758 (7)	0.0247 (2)
O5	0.12949 (6)	0.05091 (10)	0.50809 (7)	0.01987 (19)
N1	0.23857 (7)	0.21847 (11)	0.26204 (8)	0.0164 (2)
N2	0.09159 (7)	0.48102 (12)	0.57743 (8)	0.0184 (2)
N3	0.06741 (7)	0.22240 (12)	0.59639 (8)	0.0185 (2)
C1	0.26274 (9)	0.38059 (13)	0.27282 (9)	0.0182 (2)
H1A	0.2419	0.4382	0.2217	0.022*
H1B	0.3286	0.3944	0.2847	0.022*
C2	0.21053 (8)	0.42342 (13)	0.35102 (9)	0.0154 (2)
H2	0.1457	0.4359	0.3302	0.018*
C3	0.21703 (8)	0.28259 (13)	0.40731 (9)	0.0148 (2)
H3	0.2810	0.2693	0.4305	0.018*
C4	0.19337 (8)	0.16103 (13)	0.33970 (9)	0.0168 (2)
H4A	0.2185	0.0647	0.3586	0.020*
H4B	0.1273	0.1517	0.3275	0.020*
C5	0.23892 (8)	0.56320 (13)	0.40294 (9)	0.0169 (2)
C6	0.14398 (8)	0.44905 (14)	0.50888 (9)	0.0160 (2)
C7	0.15809 (8)	0.30612 (13)	0.48152 (8)	0.0151 (2)
C8	0.41258 (8)	0.09762 (14)	0.28349 (9)	0.0157 (2)
C9	0.42372 (8)	−0.01963 (13)	0.34305 (9)	0.0164 (2)
H9	0.3764	−0.0882	0.3486	0.020*
C10	0.50606 (9)	−0.03344 (14)	0.39420 (9)	0.0179 (2)
H10	0.5135	−0.1118	0.4340	0.021*
C11	0.57798 (8)	0.06859 (14)	0.38686 (9)	0.0175 (2)
C12	0.56465 (9)	0.18709 (15)	0.32874 (10)	0.0225 (3)
H12	0.6112	0.2575	0.3244	0.027*
C13	0.48266 (9)	0.20210 (15)	0.27689 (10)	0.0216 (3)
H13	0.4748	0.2817	0.2380	0.026*
C14	0.66833 (9)	0.04688 (16)	0.43953 (10)	0.0226 (3)
H14A	0.7119	0.1198	0.4223	0.034*
H14B	0.6913	−0.0521	0.4296	0.034*
H14C	0.6594	0.0591	0.5003	0.034*
C15	0.21943 (9)	0.70446 (14)	0.35015 (10)	0.0215 (3)
H15A	0.1574	0.7016	0.3243	0.032*
H15B	0.2614	0.7109	0.3051	0.032*
H15C	0.2271	0.7904	0.3875	0.032*
C16	0.33649 (9)	0.55984 (15)	0.44606 (10)	0.0237 (3)
H16A	0.3487	0.6518	0.4773	0.035*
H16B	0.3796	0.5488	0.4023	0.035*
H16C	0.3427	0.4768	0.4858	0.035*
C17	0.05352 (8)	0.36716 (15)	0.62489 (9)	0.0191 (2)
C18	0.11981 (8)	0.18359 (14)	0.52689 (9)	0.0162 (2)
C19	0.08075 (9)	0.63604 (15)	0.60710 (10)	0.0229 (3)
H19A	0.0715	0.7011	0.5575	0.034*
H19B	0.1352	0.6662	0.6418	0.034*
H19C	0.0285	0.6422	0.6414	0.034*
C20	0.02666 (10)	0.09960 (16)	0.64391 (10)	0.0238 (3)

H20A	0.0043	0.1378	0.6967	0.036*
H20B	0.0725	0.0242	0.6579	0.036*
H20C	−0.0235	0.0564	0.6083	0.036*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.01498 (13)	0.01655 (13)	0.01413 (16)	0.00030 (9)	0.00080 (10)	−0.00044 (10)
O1	0.0227 (4)	0.0243 (4)	0.0139 (5)	0.0021 (3)	0.0032 (4)	0.0016 (4)
O2	0.0184 (4)	0.0180 (4)	0.0215 (5)	−0.0012 (3)	−0.0005 (4)	−0.0032 (3)
O3	0.0231 (4)	0.0155 (4)	0.0204 (5)	−0.0011 (3)	0.0048 (4)	−0.0012 (3)
O4	0.0218 (5)	0.0345 (5)	0.0185 (5)	−0.0006 (4)	0.0051 (4)	−0.0030 (4)
O5	0.0197 (4)	0.0182 (4)	0.0218 (5)	−0.0005 (3)	0.0019 (4)	0.0029 (4)
N1	0.0164 (4)	0.0150 (4)	0.0180 (5)	−0.0001 (3)	0.0035 (4)	0.0013 (4)
N2	0.0182 (5)	0.0209 (5)	0.0161 (5)	0.0006 (4)	0.0008 (4)	−0.0033 (4)
N3	0.0172 (5)	0.0230 (5)	0.0153 (5)	−0.0020 (4)	0.0020 (4)	0.0017 (4)
C1	0.0215 (6)	0.0143 (5)	0.0193 (7)	−0.0007 (4)	0.0057 (5)	0.0020 (4)
C2	0.0155 (5)	0.0147 (5)	0.0161 (6)	−0.0004 (4)	0.0015 (4)	0.0021 (4)
C3	0.0141 (5)	0.0144 (5)	0.0160 (6)	−0.0003 (4)	0.0013 (4)	0.0015 (4)
C4	0.0169 (5)	0.0151 (5)	0.0187 (6)	−0.0009 (4)	0.0042 (4)	0.0007 (4)
C5	0.0170 (5)	0.0164 (5)	0.0177 (6)	−0.0009 (4)	0.0032 (4)	0.0006 (4)
C6	0.0153 (5)	0.0185 (5)	0.0138 (6)	−0.0006 (4)	−0.0009 (4)	0.0001 (4)
C7	0.0139 (5)	0.0169 (5)	0.0142 (6)	−0.0005 (4)	0.0002 (4)	0.0009 (4)
C8	0.0137 (5)	0.0191 (5)	0.0146 (6)	−0.0002 (4)	0.0017 (4)	−0.0003 (4)
C9	0.0169 (5)	0.0169 (5)	0.0156 (6)	−0.0015 (4)	0.0013 (4)	−0.0008 (4)
C10	0.0196 (5)	0.0184 (5)	0.0155 (6)	0.0003 (4)	0.0000 (4)	0.0003 (4)
C11	0.0142 (5)	0.0216 (5)	0.0168 (6)	0.0010 (4)	0.0011 (4)	−0.0029 (5)
C12	0.0168 (5)	0.0232 (6)	0.0275 (8)	−0.0048 (4)	0.0013 (5)	0.0029 (5)
C13	0.0178 (5)	0.0227 (6)	0.0243 (7)	−0.0026 (4)	0.0013 (5)	0.0077 (5)
C14	0.0176 (5)	0.0290 (7)	0.0207 (7)	0.0015 (5)	−0.0021 (5)	−0.0041 (5)
C15	0.0240 (6)	0.0150 (5)	0.0257 (7)	−0.0015 (4)	0.0025 (5)	0.0028 (5)
C16	0.0197 (6)	0.0221 (6)	0.0285 (8)	−0.0032 (4)	−0.0028 (5)	−0.0019 (5)
C17	0.0149 (5)	0.0274 (6)	0.0148 (6)	−0.0011 (4)	−0.0006 (4)	−0.0018 (5)
C18	0.0130 (5)	0.0212 (5)	0.0139 (6)	−0.0008 (4)	−0.0014 (4)	0.0025 (4)
C19	0.0215 (6)	0.0229 (6)	0.0240 (7)	0.0035 (4)	−0.0004 (5)	−0.0064 (5)
C20	0.0244 (6)	0.0289 (7)	0.0187 (7)	−0.0053 (5)	0.0051 (5)	0.0049 (5)

Geometric parameters (Å, °)

S1—O1	1.4350 (10)	C6—C7	1.3624 (17)
S1—O2	1.4360 (9)	C7—C18	1.4318 (17)
S1—N1	1.6228 (11)	C8—C13	1.3910 (17)
S1—C8	1.7639 (13)	C8—C9	1.3919 (18)
O3—C6	1.3384 (15)	C9—C10	1.3894 (18)
O3—C5	1.4812 (16)	C9—H9	0.93
O4—C17	1.2238 (16)	C10—C11	1.3980 (17)
O5—C18	1.2283 (15)	C10—H10	0.93
N1—C1	1.4938 (16)	C11—C12	1.3886 (19)
N1—C4	1.4977 (16)	C11—C14	1.5051 (18)

N2—C6	1.3778 (17)	C12—C13	1.3917 (19)
N2—C17	1.3901 (17)	C12—H12	0.93
N2—C19	1.4677 (17)	C13—H13	0.93
N3—C17	1.3827 (17)	C14—H14A	0.96
N3—C18	1.4035 (17)	C14—H14B	0.96
N3—C20	1.4666 (17)	C14—H14C	0.96
C1—C2	1.5202 (18)	C15—H15A	0.96
C1—H1A	0.97	C15—H15B	0.96
C1—H1B	0.97	C15—H15C	0.96
C2—C5	1.5207 (17)	C16—H16A	0.96
C2—C3	1.5244 (17)	C16—H16B	0.96
C2—H2	0.98	C16—H16C	0.96
C3—C7	1.4945 (17)	C19—H19A	0.96
C3—C4	1.5240 (18)	C19—H19B	0.96
C3—H3	0.98	C19—H19C	0.96
C4—H4A	0.97	C20—H20A	0.96
C4—H4B	0.97	C20—H20B	0.96
C5—C15	1.5140 (18)	C20—H20C	0.96
C5—C16	1.5225 (18)		
O1—S1—O2	120.33 (6)	C13—C8—S1	119.58 (10)
O1—S1—N1	106.40 (6)	C9—C8—S1	120.33 (9)
O2—S1—N1	107.02 (5)	C10—C9—C8	119.52 (11)
O1—S1—C8	106.89 (6)	C10—C9—H9	120.2
O2—S1—C8	107.27 (6)	C8—C9—H9	120.2
N1—S1—C8	108.52 (6)	C9—C10—C11	121.07 (12)
C6—O3—C5	119.64 (10)	C9—C10—H10	119.5
C1—N1—C4	110.86 (10)	C11—C10—H10	119.5
C1—N1—S1	117.16 (8)	C12—C11—C10	118.55 (12)
C4—N1—S1	119.89 (8)	C12—C11—C14	121.27 (12)
C6—N2—C17	121.15 (11)	C10—C11—C14	120.16 (12)
C6—N2—C19	120.79 (11)	C11—C12—C13	121.00 (12)
C17—N2—C19	117.87 (11)	C11—C12—H12	119.5
C17—N3—C18	124.95 (11)	C13—C12—H12	119.5
C17—N3—C20	117.64 (11)	C8—C13—C12	119.74 (12)
C18—N3—C20	117.38 (11)	C8—C13—H13	120.1
N1—C1—C2	101.73 (9)	C12—C13—H13	120.1
N1—C1—H1A	111.4	C11—C14—H14A	109.5
C2—C1—H1A	111.4	C11—C14—H14B	109.5
N1—C1—H1B	111.4	H14A—C14—H14B	109.5
C2—C1—H1B	111.4	C11—C14—H14C	109.5
H1A—C1—H1B	109.3	H14A—C14—H14C	109.5
C1—C2—C5	119.32 (10)	H14B—C14—H14C	109.5
C1—C2—C3	103.30 (9)	C5—C15—H15A	109.5
C5—C2—C3	111.91 (11)	C5—C15—H15B	109.5
C1—C2—H2	107.2	H15A—C15—H15B	109.5
C5—C2—H2	107.2	C5—C15—H15C	109.5
C3—C2—H2	107.2	H15A—C15—H15C	109.5
C7—C3—C4	120.58 (10)	H15B—C15—H15C	109.5
C7—C3—C2	107.72 (10)	C5—C16—H16A	109.5

C4—C3—C2	101.31 (10)	C5—C16—H16B	109.5
C7—C3—H3	108.9	H16A—C16—H16B	109.5
C4—C3—H3	108.9	C5—C16—H16C	109.5
C2—C3—H3	108.9	H16A—C16—H16C	109.5
N1—C4—C3	102.24 (9)	H16B—C16—H16C	109.5
N1—C4—H4A	111.3	O4—C17—N3	122.63 (12)
C3—C4—H4A	111.3	O4—C17—N2	121.19 (12)
N1—C4—H4B	111.3	N3—C17—N2	116.17 (12)
C3—C4—H4B	111.3	O5—C18—N3	119.71 (11)
H4A—C4—H4B	109.2	O5—C18—C7	124.32 (12)
O3—C5—C15	103.82 (10)	N3—C18—C7	115.96 (11)
O3—C5—C2	106.47 (9)	N2—C19—H19A	109.5
C15—C5—C2	111.51 (11)	N2—C19—H19B	109.5
O3—C5—C16	106.80 (11)	H19A—C19—H19B	109.5
C15—C5—C16	112.43 (10)	N2—C19—H19C	109.5
C2—C5—C16	114.89 (10)	H19A—C19—H19C	109.5
O3—C6—C7	126.20 (12)	H19B—C19—H19C	109.5
O3—C6—N2	111.42 (11)	N3—C20—H20A	109.5
C7—C6—N2	122.36 (11)	N3—C20—H20B	109.5
C6—C7—C18	119.30 (12)	H20A—C20—H20B	109.5
C6—C7—C3	118.44 (11)	N3—C20—H20C	109.5
C18—C7—C3	122.20 (11)	H20A—C20—H20C	109.5
C13—C8—C9	120.07 (12)	H20B—C20—H20C	109.5
O1—S1—N1—C1	−46.84 (11)	C4—C3—C7—C6	−142.71 (12)
O2—S1—N1—C1	−176.68 (9)	C2—C3—C7—C6	−27.39 (15)
C8—S1—N1—C1	67.86 (11)	C4—C3—C7—C18	40.19 (17)
O1—S1—N1—C4	174.01 (9)	C2—C3—C7—C18	155.52 (11)
O2—S1—N1—C4	44.17 (11)	O1—S1—C8—C13	25.07 (12)
C8—S1—N1—C4	−71.29 (10)	O2—S1—C8—C13	155.40 (11)
C4—N1—C1—C2	−12.07 (13)	N1—S1—C8—C13	−89.30 (12)
S1—N1—C1—C2	−154.71 (9)	O1—S1—C8—C9	−153.79 (10)
N1—C1—C2—C5	160.36 (11)	O2—S1—C8—C9	−23.47 (12)
N1—C1—C2—C3	35.44 (12)	N1—S1—C8—C9	91.83 (11)
C1—C2—C3—C7	−173.40 (10)	C13—C8—C9—C10	−1.55 (19)
C5—C2—C3—C7	57.00 (12)	S1—C8—C9—C10	177.31 (10)
C1—C2—C3—C4	−45.92 (11)	C8—C9—C10—C11	0.01 (19)
C5—C2—C3—C4	−175.53 (9)	C9—C10—C11—C12	1.7 (2)
C1—N1—C4—C3	−15.84 (12)	C9—C10—C11—C14	−176.80 (12)
S1—N1—C4—C3	125.64 (9)	C10—C11—C12—C13	−1.9 (2)
C7—C3—C4—N1	155.66 (10)	C14—C11—C12—C13	176.59 (13)
C2—C3—C4—N1	37.06 (11)	C9—C8—C13—C12	1.4 (2)
C6—O3—C5—C15	150.57 (11)	S1—C8—C13—C12	−177.51 (11)
C6—O3—C5—C2	32.76 (14)	C11—C12—C13—C8	0.4 (2)
C6—O3—C5—C16	−90.44 (13)	C18—N3—C17—O4	−177.69 (12)
C1—C2—C5—O3	−179.96 (10)	C20—N3—C17—O4	0.39 (19)
C3—C2—C5—O3	−59.28 (12)	C18—N3—C17—N2	3.09 (18)
C1—C2—C5—C15	67.44 (14)	C20—N3—C17—N2	−178.83 (11)
C3—C2—C5—C15	−171.88 (10)	C6—N2—C17—O4	177.54 (12)
C1—C2—C5—C16	−61.97 (16)	C19—N2—C17—O4	2.55 (19)

C3—C2—C5—C16	58.71 (14)	C6—N2—C17—N3	−3.23 (18)
C5—O3—C6—C7	−5.18 (19)	C19—N2—C17—N3	−178.23 (11)
C5—O3—C6—N2	176.01 (10)	C17—N3—C18—O5	178.37 (12)
C17—N2—C6—O3	−178.26 (11)	C20—N3—C18—O5	0.29 (17)
C19—N2—C6—O3	−3.41 (17)	C17—N3—C18—C7	−2.33 (18)
C17—N2—C6—C7	2.88 (19)	C20—N3—C18—C7	179.59 (11)
C19—N2—C6—C7	177.73 (12)	C6—C7—C18—O5	−179.08 (12)
O3—C6—C7—C18	179.29 (12)	C3—C7—C18—O5	−2.02 (19)
N2—C6—C7—C18	−2.02 (19)	C6—C7—C18—N3	1.65 (17)
O3—C6—C7—C3	2.11 (19)	C3—C7—C18—N3	178.72 (11)
N2—C6—C7—C3	−179.20 (11)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15A···O4^{i}	0.96	2.57	3.4571 (17)	153
C20—H20C···O5^{ii}	0.96	2.47	3.4125 (18)	168
C19—H19B···O2^{iii}	0.96	2.44	3.1917 (17)	134
C14—H14B···O1^{iv}	0.96	2.52	3.3787 (17)	149

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

Fig. 1

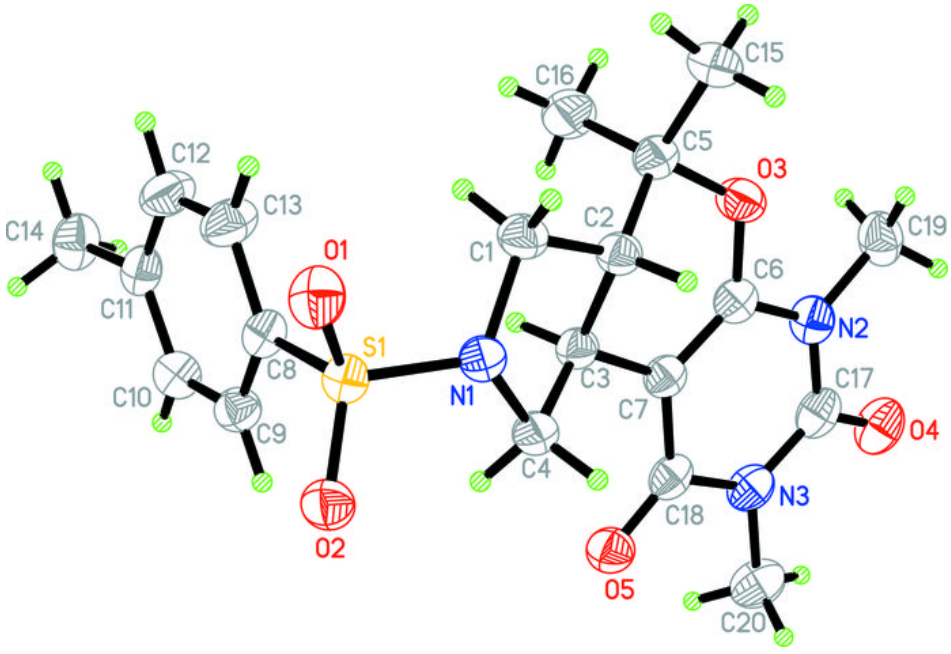

C15
C16
C5
O3
C19
C12
C13
C2
C14
O1
C1
C6
N2
C11
S1
C8
N1
C3
C7
C17
O4
C10
C9
C4
N3
C18
O2
O5
C20

Fig. 2

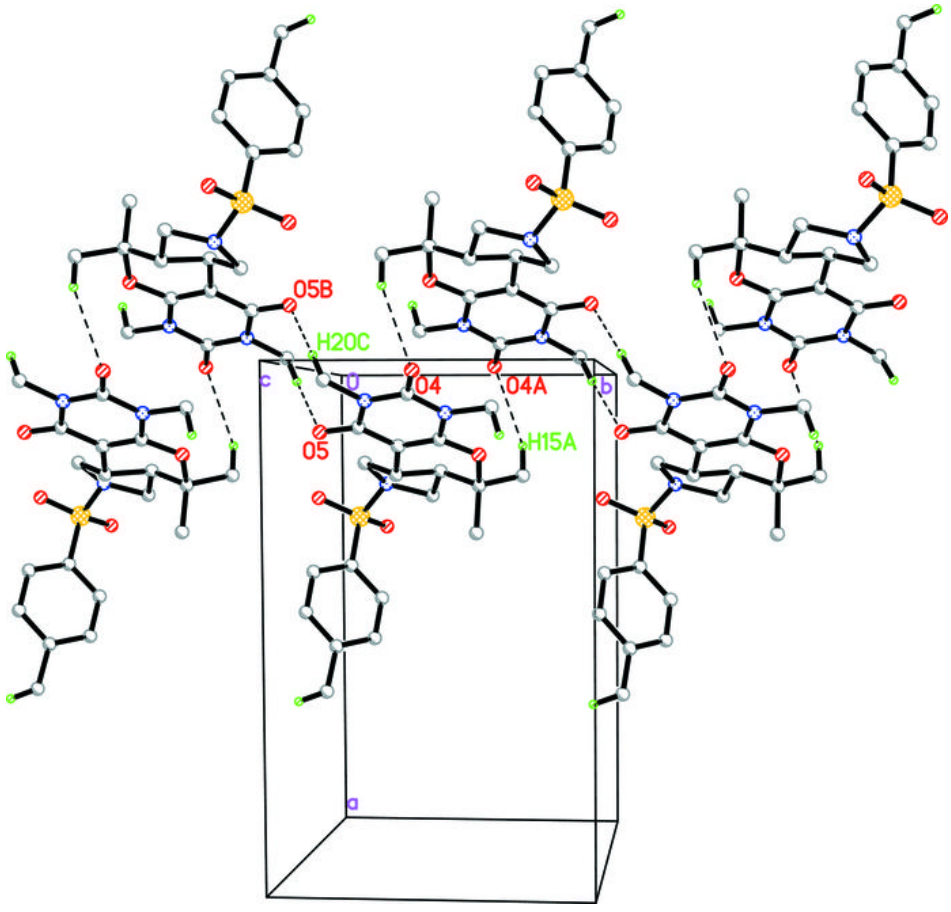
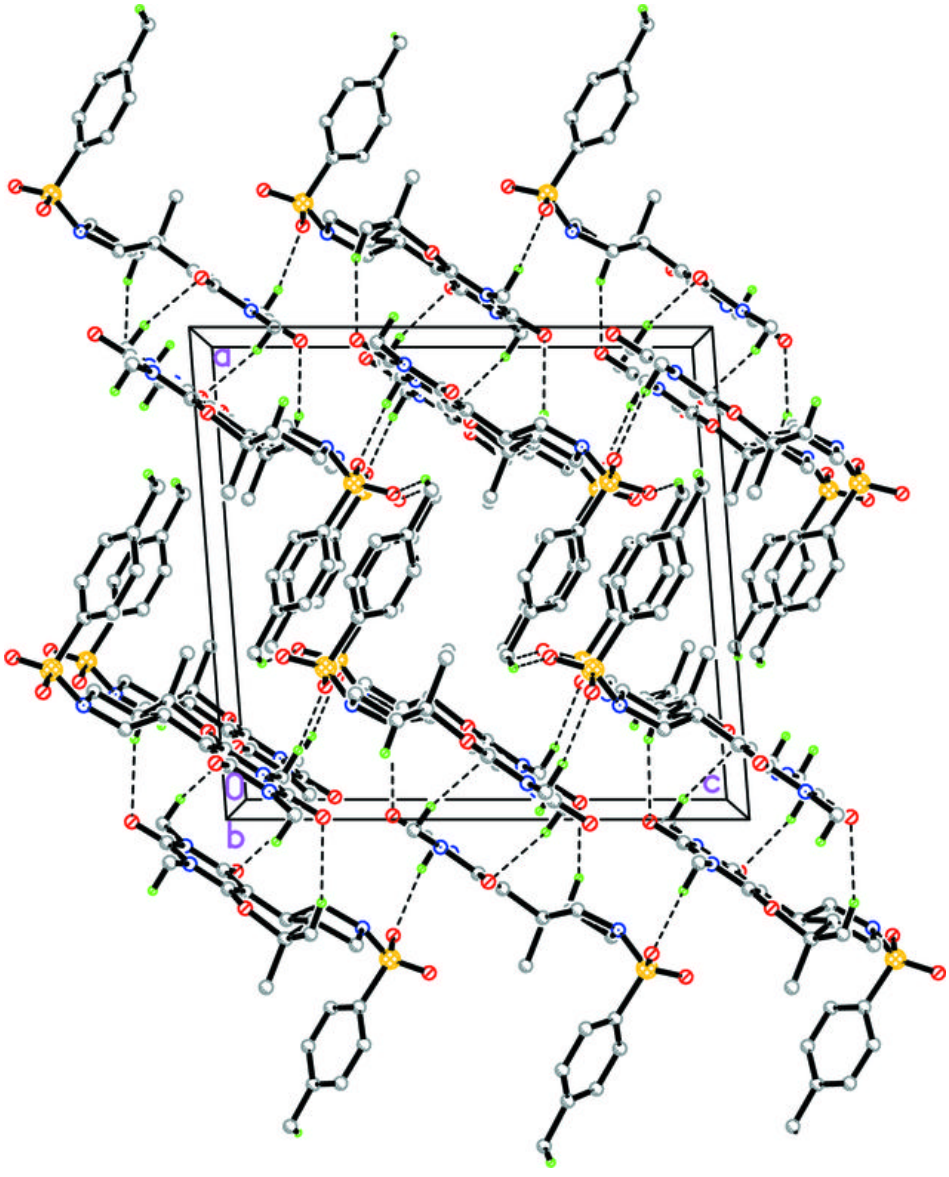


Fig. 3



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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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