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

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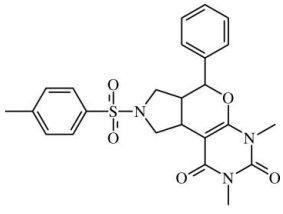
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.047; wR factor = 0.138; data-to-parameter ratio = 31.8.

In the title compound, $C_{24}H_{25}N_3O_5S$, both the pyrrolidine and dihydropyran rings adopt envelope conformations, and are *cis*-fused. The tosyl group is equatorially attached to the pyrrolidine ring. The glide-related molecules are linked by C—H···O hydrogen bonds, forming a $C(6)$ chain along the c axis, and adjacent chains are cross-linked *via* C—H···O and C—H···π interactions, forming a two-dimensional network parallel to the bc plane.

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 bond-length data, see: Allen *et al.* (1987). For ring puckering parameters, see: Cremer & Pople (1975). For asymmetry parameters, see: Duax *et al.* (1976).



Experimental

Crystal data

$C_{24}H_{25}N_3O_5S$ M_r = 467.53
Monoclinic, $P2_1/c$
a = 16.2810 (2) Å
b = 8.4063 (1) Å
c = 16.0030 (2) Å
β = 93.400 (1)°
V = 2186.36 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.19 mm^{-1}
T = 100.0 (1) K
0.42 × 0.19 × 0.18 mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.924, T_{max} = 0.967
40900 measured reflections
9583 independent reflections
7316 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.138
S = 1.06
9583 reflections
301 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.68 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

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

Cg1 is the centroid of the C8–C13 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10···O1^{i}	0.93	2.46	3.1846 (14)	134
C18—H18···O4^{ii}	0.93	2.47	3.2248 (15)	138
C20—H20···*Cg1*^{iii}	0.93	2.77	3.6038 (13)	149

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

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: IS2222).

References

Abdel Fattah, M. E., Atta, A. H., Abdel Gawad, I. I. & Mina, S. M. (2004). *Orient. J. Chem.* **20**, 257–262.
Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–S19.
Bedair, A. H., El-Hady, N. A., El-Latif, A., Fakery, A. H. & El-Agrody, A. M. (2000). *Farmaco*, **55**, 708–714.
Bedair, A. H., Emam, H. A., El-Hady, N. A., Ahmed, K. A. & El-Agrody, A. M. (2001). *Farmaco*, **56**, 965–973.
Bruker (2005). *APEX2* (Version 1.27), *SAINT* (Version 7.12a) and *SADABS* (Version 2004/1). Bruker AXS Inc., Madison, Wisconsin, USA.
Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.
Duax, W. L., Weeks, C. M. & Rohrer, D. C. (1976). *Topics in Stereochemistry*, Vol. 9, edited by E. L. Eliel & N. L. Allinger, pp. 271–383. New York: John Wiley.
Eid, F. A., Abd El-Wahab, A. H., Ali, G. A. & Khafagy, M. M. (2004). *Acta Pharm.* **54**, 13–26.
Shamroukh, A. H., Zaki, M. E., Morsy, E. M., Abdel-Motti, F. M. & Abdel-Megeid, F. M. (2007). *Arch. Pharm. (Weinheim)*, **340**, 236–343.
Sheldrick, G. M. (1998). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

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supplementary materials

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6,8-Dimethyl-4-phenyl-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 title molecule, all geometric parameters show normal values (Allen *et al.*, 1987). The significant widening of the O1—S1—O2 [120.49 (6)°] angle from the ideal tetrahedral value is the result of the non-bonding interactions between the short S═O bonds. The sum of the angles around the pyrrolidine N atom (348.3 °) indicates sp^3-hybridization.

The pyrrolidine ring has an envelope conformation, with C1, the envelope flap, lying 0.573 (2) Å from the plane defined by C2, C3, C4 and N1 atoms. The Cremer and Pople puckering parameters (Cremer & Pople, 1975) are q = 0.374 (1) Å and φ = 219.9 (2)°; the asymmetry parameter (Duax *et al.*, 1976) ΔC_s[C1] is 1.6 (1)°. The tosyl group is equatorially attached to the pyrrolidine ring.

The dihydropyran ring (O3/C5/C2/C3/C7/C6) also adopts an enveope conformation, with atom C5 deviating from the O3/C2/C3/C7/C6 plane by 0.655 (2) Å; the lowest asymmetry parameter is ΔC_s[C5] = 7.7 (1)°, and the puckering parameters Q, θ and φ are 0.480 (1) Å, 123.4 (1)° and 252.4 (2)°, respectively. The phenyl ring is equatorially attached to the dihydropyran ring.

The C2—C4/N1 plane forms dihedral angles of 55.26 (5) and 84.93 (4)°, respectively, with the O3/C2/C3/C7/C6 and C8—C13 planes. The O3/C2/C3/C7/C6 plane forms dihedral angles of 7.04 (6) and 74.98 (4)°, respectively, with the pyrimidine (C7/C6/N2/C15/N3/C16) and pheny (C17—C22) planes. Atoms O4, O5, C23 and C24 deviate from the pyrimidine ring plane by 0.101 (2), 0.009 (2), 0.149 (2) and −0.072 (2) Å, respectively.

The glide-related molecules are linked to form a C(6) chain along the *c* axis by C10—H10···O1^{i} hydrogen bonds. The molecules of the adjacent chains are cross-linked *via* C18—H18···O4^{ii} and C20—H20···*Cg*1^{iii} (*Cg*1 is the C8—C13 ring centroid) interactions, forming a two-dimensional network parallel to the *bc* plane (Fig. 2). In the network, pairs of C18—H18···O4 hydrogen bonds generate $R^2_2(18)$ ring motif.

Experimental

To a solution of 1,3-dimethyl-pyrimidine-2,4,6-trione (1 mmol) in dry toluene (20 ml), the corresponding 2-(*N*-cinnamyl-*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 and constrained to ride on their parent atoms [for methyl H atoms, C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C), for aromatic C—H = 0.93 Å and methine C—H = 0.98 Å, and U_{iso}(H) = 1.2U_{eq}(C)]. A rotating group model was used for the methyl groups attached to aromatic rings.

Figures

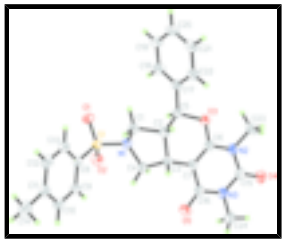


Fig. 1. The molecular structure of the title compound, showing 80% probability displacement ellipsoids and the atomic numbering.

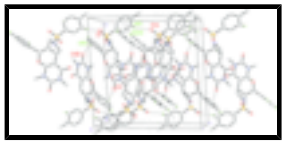


Fig. 2. The crystal packing of the title compound, viewed approximately along the *b* axis. Dashed and dotted lines indicate C—H···O and C—H···π interactions, respectively. For the sake of clarity, H atoms not involved in the interactions have been omitted. Atoms labelled with the suffixes A, B and C are generated by the symmetry operations (x, 3/2 − y, 1/2 + z), (1 − x, 1 − y, −z) and (x, 1/2 − y, 1/2 + z), respectively.

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

Crystal data

$C_{24}H_{25}N_3O_5S$	F_{000} = 984
M_r = 467.53	D_x = 1.420 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 8951 reflections
a = 16.2810 (2) Å	θ = 2.5–34.9º
b = 8.4063 (1) Å	μ = 0.19 mm^{-1}
c = 16.0030 (2) Å	T = 100.0 (1) K
β = 93.400 (1)º	Block, colourless
V = 2186.36 (5) Å^3	0.42 × 0.19 × 0.18 mm
Z = 4	

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer	9583 independent reflections
Radiation source: fine-focus sealed tube	7316 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.045
Detector resolution: 8.33 pixels mm^{-1}	θ_{max} = 35.0º
T = 100.0(1) K	θ_{min} = 1.3º
ω scans	h = −26→26

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

T_{min} = 0.924, T_{max} = 0.967

40900 measured reflections

k = −12→13

l = −25→25

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.047

$wR(F^2)$ = 0.138

S = 1.06

9583 reflections

301 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

$w = 1/[\sigma^2(F_o^2) + (0.0688P)^2 + 0.5404P]$ where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max}$ = 0.68 e Å^{-3}

$\Delta\rho_{min}$ = −0.46 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	0.832515 (17)	0.76601 (4)	0.138778 (16)	0.01501 (7)
O1	0.88386 (6)	0.74316 (12)	0.07011 (5)	0.02264 (19)
O2	0.78444 (6)	0.90866 (11)	0.14475 (5)	0.01949 (17)
O3	0.59556 (5)	0.28693 (11)	0.03949 (5)	0.01591 (15)
O4	0.33422 (5)	0.33580 (11)	0.12096 (6)	0.01933 (17)
O5	0.53895 (6)	0.56887 (12)	0.28523 (6)	0.02265 (19)
N1	0.76755 (6)	0.61871 (12)	0.13603 (6)	0.01536 (17)
N2	0.46544 (6)	0.31994 (12)	0.07934 (6)	0.01493 (17)
N3	0.43589 (6)	0.46118 (12)	0.20054 (6)	0.01647 (18)
C1	0.79886 (7)	0.45520 (14)	0.12820 (7)	0.0164 (2)
H1A	0.8357	0.4266	0.1757	0.020*
H1B	0.8272	0.4417	0.0770	0.020*
C2	0.71959 (7)	0.35804 (14)	0.12631 (7)	0.01415 (19)

H2	0.7309	0.2489	0.1452	0.017*
C3	0.66682 (7)	0.44598 (13)	0.18863 (7)	0.01388 (18)
H3	0.6778	0.3984	0.2441	0.017*
C4	0.69846 (7)	0.61972 (14)	0.19205 (7)	0.01552 (19)
H4A	0.6558	0.6932	0.1720	0.019*
H4B	0.7172	0.6491	0.2486	0.019*
C5	0.67726 (6)	0.35828 (13)	0.03792 (7)	0.01347 (18)
H5	0.6717	0.4683	0.0182	0.016*
C6	0.54775 (7)	0.34867 (13)	0.09687 (7)	0.01378 (18)
C7	0.57664 (7)	0.43028 (13)	0.16549 (7)	0.01420 (19)
C8	0.89543 (7)	0.74930 (13)	0.23173 (7)	0.01382 (19)
C9	0.86994 (7)	0.81965 (14)	0.30474 (7)	0.01478 (19)
H9	0.8205	0.8753	0.3042	0.018*
C10	0.91903 (7)	0.80569 (15)	0.37815 (7)	0.0167 (2)
H10	0.9023	0.8528	0.4269	0.020*
C11	0.99333 (7)	0.72184 (15)	0.38006 (7)	0.0172 (2)
C12	1.01751 (7)	0.65221 (15)	0.30632 (8)	0.0193 (2)
H12	1.0667	0.5957	0.3069	0.023*
C13	0.96929 (7)	0.66587 (15)	0.23177 (7)	0.0177 (2)
H13	0.9862	0.6199	0.1828	0.021*
C14	1.04485 (8)	0.70532 (19)	0.46063 (8)	0.0254 (3)
H14A	1.0955	0.6527	0.4501	0.038*
H14B	1.0155	0.6438	0.4996	0.038*
H14C	1.0565	0.8089	0.4837	0.038*
C15	0.40695 (7)	0.36841 (13)	0.13370 (7)	0.01505 (19)
C16	0.51885 (7)	0.49219 (14)	0.22172 (7)	0.0161 (2)
C17	0.72352 (7)	0.26413 (13)	−0.02389 (7)	0.01317 (18)
C18	0.76919 (7)	0.34268 (14)	−0.08228 (7)	0.0167 (2)
H18	0.7678	0.4531	−0.0856	0.020*
C19	0.81689 (8)	0.25623 (15)	−0.13557 (7)	0.0184 (2)
H19	0.8474	0.3090	−0.1743	0.022*
C20	0.81894 (7)	0.09128 (15)	−0.13105 (7)	0.0181 (2)
H20	0.8515	0.0338	−0.1662	0.022*
C21	0.77236 (8)	0.01197 (15)	−0.07405 (7)	0.0184 (2)
H21	0.7727	−0.0986	−0.0719	0.022*
C22	0.72519 (7)	0.09827 (14)	−0.02033 (7)	0.0163 (2)
H22	0.6946	0.0451	0.0182	0.020*
C23	0.43769 (8)	0.21169 (17)	0.01139 (8)	0.0220 (2)
H23A	0.4714	0.2259	−0.0352	0.033*
H23B	0.3814	0.2346	−0.0057	0.033*
H23C	0.4421	0.1037	0.0307	0.033*
C24	0.37563 (7)	0.52532 (16)	0.25595 (8)	0.0217 (2)
H24A	0.3229	0.4778	0.2425	0.033*
H24B	0.3717	0.6385	0.2487	0.033*
H24C	0.3927	0.5018	0.3130	0.033*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.01520 (12)	0.01894 (13)	0.01099 (11)	−0.00379 (10)	0.00169 (8)	0.00011 (9)
O1	0.0219 (4)	0.0333 (5)	0.0132 (4)	−0.0083 (4)	0.0058 (3)	−0.0025 (3)
O2	0.0211 (4)	0.0187 (4)	0.0183 (4)	−0.0010 (3)	−0.0017 (3)	0.0041 (3)
O3	0.0121 (3)	0.0194 (4)	0.0163 (4)	−0.0016 (3)	0.0014 (3)	−0.0051 (3)
O4	0.0121 (3)	0.0194 (4)	0.0263 (4)	0.0000 (3)	−0.0002 (3)	−0.0009 (3)
O5	0.0180 (4)	0.0287 (5)	0.0215 (4)	−0.0032 (4)	0.0029 (3)	−0.0104 (3)
N1	0.0138 (4)	0.0168 (4)	0.0157 (4)	−0.0024 (3)	0.0028 (3)	−0.0028 (3)
N2	0.0117 (4)	0.0159 (4)	0.0170 (4)	−0.0006 (3)	−0.0004 (3)	−0.0023 (3)
N3	0.0126 (4)	0.0167 (4)	0.0204 (4)	−0.0006 (3)	0.0037 (3)	−0.0042 (3)
C1	0.0125 (4)	0.0192 (5)	0.0173 (5)	−0.0010 (4)	0.0010 (4)	−0.0051 (4)
C2	0.0129 (4)	0.0154 (5)	0.0140 (4)	0.0004 (4)	0.0003 (3)	−0.0011 (3)
C3	0.0127 (4)	0.0165 (5)	0.0124 (4)	−0.0010 (4)	0.0010 (3)	−0.0018 (3)
C4	0.0129 (4)	0.0164 (5)	0.0175 (5)	−0.0023 (4)	0.0031 (4)	−0.0032 (4)
C5	0.0120 (4)	0.0145 (4)	0.0140 (4)	−0.0006 (4)	0.0012 (3)	−0.0012 (3)
C6	0.0122 (4)	0.0140 (4)	0.0152 (4)	−0.0003 (4)	0.0012 (3)	−0.0007 (3)
C7	0.0122 (4)	0.0151 (5)	0.0154 (4)	−0.0012 (4)	0.0011 (3)	−0.0020 (4)
C8	0.0128 (4)	0.0153 (5)	0.0135 (4)	−0.0026 (4)	0.0022 (3)	−0.0007 (3)
C9	0.0146 (4)	0.0163 (5)	0.0136 (4)	0.0008 (4)	0.0025 (3)	−0.0005 (4)
C10	0.0170 (5)	0.0205 (5)	0.0128 (4)	−0.0003 (4)	0.0018 (4)	−0.0004 (4)
C11	0.0144 (4)	0.0203 (5)	0.0169 (5)	−0.0029 (4)	0.0003 (4)	0.0035 (4)
C12	0.0144 (5)	0.0193 (5)	0.0244 (5)	0.0015 (4)	0.0018 (4)	0.0006 (4)
C13	0.0149 (4)	0.0200 (5)	0.0187 (5)	−0.0004 (4)	0.0036 (4)	−0.0043 (4)
C14	0.0166 (5)	0.0388 (8)	0.0204 (6)	−0.0009 (5)	−0.0026 (4)	0.0075 (5)
C15	0.0130 (4)	0.0124 (4)	0.0197 (5)	0.0010 (4)	0.0013 (4)	0.0002 (4)
C16	0.0142 (4)	0.0159 (5)	0.0185 (5)	−0.0015 (4)	0.0024 (4)	−0.0026 (4)
C17	0.0131 (4)	0.0141 (4)	0.0122 (4)	0.0004 (4)	−0.0002 (3)	−0.0010 (3)
C18	0.0187 (5)	0.0155 (5)	0.0161 (5)	0.0011 (4)	0.0028 (4)	0.0012 (4)
C19	0.0190 (5)	0.0212 (5)	0.0154 (5)	0.0019 (4)	0.0043 (4)	0.0011 (4)
C20	0.0191 (5)	0.0205 (5)	0.0146 (5)	0.0031 (4)	0.0002 (4)	−0.0043 (4)
C21	0.0211 (5)	0.0155 (5)	0.0185 (5)	0.0010 (4)	0.0001 (4)	−0.0033 (4)
C22	0.0179 (5)	0.0146 (5)	0.0163 (5)	−0.0007 (4)	0.0011 (4)	−0.0009 (4)
C23	0.0158 (5)	0.0243 (6)	0.0252 (6)	−0.0011 (4)	−0.0029 (4)	−0.0103 (5)
C24	0.0157 (5)	0.0225 (6)	0.0275 (6)	−0.0003 (4)	0.0066 (4)	−0.0067 (5)

Geometric parameters (Å, °)

S1—O1	1.4325 (9)	C8—C13	1.3920 (16)
S1—O2	1.4383 (10)	C8—C9	1.3944 (15)
S1—N1	1.6274 (10)	C9—C10	1.3862 (16)
S1—C8	1.7610 (11)	C9—H9	0.93
O3—C6	1.3430 (13)	C10—C11	1.3988 (17)
O3—C5	1.4606 (13)	C10—H10	0.93
O4—C15	1.2208 (13)	C11—C12	1.3947 (18)
O5—C16	1.2312 (14)	C11—C14	1.5023 (17)
N1—C1	1.4740 (15)	C12—C13	1.3935 (17)

N1—C4	1.4793 (14)	C12—H12	0.93
N2—C6	1.3741 (14)	C13—H13	0.93
N2—C15	1.3883 (15)	C14—H14A	0.96
N2—C23	1.4685 (15)	C14—H14B	0.96
N3—C15	1.3837 (15)	C14—H14C	0.96
N3—C16	1.3975 (15)	C17—C18	1.3945 (15)
N3—C24	1.4637 (15)	C17—C22	1.3956 (16)
C1—C2	1.5262 (16)	C18—C19	1.3918 (16)
C1—H1A	0.97	C18—H18	0.93
C1—H1B	0.97	C19—C20	1.3888 (18)
C2—C5	1.5362 (15)	C19—H19	0.93
C2—C3	1.5430 (15)	C20—C21	1.3907 (17)
C2—H2	0.98	C20—H20	0.93
C3—C7	1.4985 (15)	C21—C22	1.3904 (16)
C3—C4	1.5486 (16)	C21—H21	0.93
C3—H3	0.98	C22—H22	0.93
C4—H4A	0.97	C23—H23A	0.96
C4—H4B	0.97	C23—H23B	0.96
C5—C17	1.5035 (15)	C23—H23C	0.96
C5—H5	0.98	C24—H24A	0.96
C6—C7	1.3552 (15)	C24—H24B	0.96
C7—C16	1.4375 (15)	C24—H24C	0.96
O1—S1—O2	120.49 (6)	C10—C9—H9	120.4
O1—S1—N1	106.57 (5)	C8—C9—H9	120.4
O2—S1—N1	106.31 (5)	C9—C10—C11	121.04 (11)
O1—S1—C8	107.50 (5)	C9—C10—H10	119.5
O2—S1—C8	107.58 (5)	C11—C10—H10	119.5
N1—S1—C8	107.86 (5)	C12—C11—C10	118.69 (11)
C6—O3—C5	114.73 (8)	C12—C11—C14	121.07 (11)
C1—N1—C4	109.64 (9)	C10—C11—C14	120.23 (11)
C1—N1—S1	118.97 (8)	C13—C12—C11	121.12 (11)
C4—N1—S1	119.71 (8)	C13—C12—H12	119.4
C6—N2—C15	121.15 (9)	C11—C12—H12	119.4
C6—N2—C23	120.90 (9)	C8—C13—C12	118.99 (11)
C15—N2—C23	116.98 (9)	C8—C13—H13	120.5
C15—N3—C16	124.92 (9)	C12—C13—H13	120.5
C15—N3—C24	117.79 (9)	C11—C14—H14A	109.5
C16—N3—C24	117.21 (10)	C11—C14—H14B	109.5
N1—C1—C2	101.79 (9)	H14A—C14—H14B	109.5
N1—C1—H1A	111.4	C11—C14—H14C	109.5
C2—C1—H1A	111.4	H14A—C14—H14C	109.5
N1—C1—H1B	111.4	H14B—C14—H14C	109.5
C2—C1—H1B	111.4	O4—C15—N3	122.55 (10)
H1A—C1—H1B	109.3	O4—C15—N2	121.59 (10)
C1—C2—C5	110.50 (9)	N3—C15—N2	115.79 (9)
C1—C2—C3	103.50 (9)	O5—C16—N3	120.23 (10)
C5—C2—C3	110.97 (9)	O5—C16—C7	123.68 (10)
C1—C2—H2	110.6	N3—C16—C7	116.09 (10)
C5—C2—H2	110.6	C18—C17—C22	119.37 (10)

C3—C2—H2	110.6	C18—C17—C5	119.96 (10)
C7—C3—C2	111.90 (9)	C22—C17—C5	120.56 (10)
C7—C3—C4	114.26 (9)	C19—C18—C17	120.16 (11)
C2—C3—C4	106.13 (9)	C19—C18—H18	119.9
C7—C3—H3	108.1	C17—C18—H18	119.9
C2—C3—H3	108.1	C20—C19—C18	120.13 (11)
C4—C3—H3	108.1	C20—C19—H19	119.9
N1—C4—C3	103.68 (9)	C18—C19—H19	119.9
N1—C4—H4A	111.0	C19—C20—C21	120.03 (11)
C3—C4—H4A	111.0	C19—C20—H20	120.0
N1—C4—H4B	111.0	C21—C20—H20	120.0
C3—C4—H4B	111.0	C22—C21—C20	119.87 (11)
H4A—C4—H4B	109.0	C22—C21—H21	120.1
O3—C5—C17	106.69 (9)	C20—C21—H21	120.1
O3—C5—C2	110.06 (9)	C21—C22—C17	120.41 (11)
C17—C5—C2	112.97 (9)	C21—C22—H22	119.8
O3—C5—H5	109.0	C17—C22—H22	119.8
C17—C5—H5	109.0	N2—C23—H23A	109.5
C2—C5—H5	109.0	N2—C23—H23B	109.5
O3—C6—C7	124.21 (10)	H23A—C23—H23B	109.5
O3—C6—N2	112.98 (9)	N2—C23—H23C	109.5
C7—C6—N2	122.81 (10)	H23A—C23—H23C	109.5
C6—C7—C16	118.81 (10)	H23B—C23—H23C	109.5
C6—C7—C3	122.19 (10)	N3—C24—H24A	109.5
C16—C7—C3	118.78 (9)	N3—C24—H24B	109.5
C13—C8—C9	120.89 (10)	H24A—C24—H24B	109.5
C13—C8—S1	119.98 (8)	N3—C24—H24C	109.5
C9—C8—S1	119.13 (8)	H24A—C24—H24C	109.5
C10—C9—C8	119.26 (10)	H24B—C24—H24C	109.5
O1—S1—N1—C1	49.11 (10)	O1—S1—C8—C9	157.46 (9)
O2—S1—N1—C1	178.80 (8)	O2—S1—C8—C9	26.32 (11)
C8—S1—N1—C1	−66.07 (9)	N1—S1—C8—C9	−87.98 (10)
O1—S1—N1—C4	−171.57 (9)	C13—C8—C9—C10	−0.09 (17)
O2—S1—N1—C4	−41.89 (10)	S1—C8—C9—C10	179.52 (9)
C8—S1—N1—C4	73.25 (10)	C8—C9—C10—C11	−0.24 (18)
C4—N1—C1—C2	38.03 (11)	C9—C10—C11—C12	0.12 (18)
S1—N1—C1—C2	−178.92 (7)	C9—C10—C11—C14	−178.78 (12)
N1—C1—C2—C5	81.66 (10)	C10—C11—C12—C13	0.33 (18)
N1—C1—C2—C3	−37.21 (10)	C14—C11—C12—C13	179.23 (12)
C1—C2—C3—C7	149.83 (9)	C9—C8—C13—C12	0.53 (17)
C5—C2—C3—C7	31.29 (13)	S1—C8—C13—C12	−179.07 (9)
C1—C2—C3—C4	24.58 (11)	C11—C12—C13—C8	−0.65 (18)
C5—C2—C3—C4	−93.96 (10)	C16—N3—C15—O4	174.90 (11)
C1—N1—C4—C3	−22.41 (11)	C24—N3—C15—O4	−1.82 (17)
S1—N1—C4—C3	−165.14 (8)	C16—N3—C15—N2	−7.87 (17)
C7—C3—C4—N1	−126.07 (9)	C24—N3—C15—N2	175.41 (10)
C2—C3—C4—N1	−2.28 (11)	C6—N2—C15—O4	−175.92 (11)
C6—O3—C5—C17	174.84 (9)	C23—N2—C15—O4	−7.14 (17)
C6—O3—C5—C2	51.94 (12)	C6—N2—C15—N3	6.82 (16)

C1—C2—C5—O3	−171.08 (9)	C23—N2—C15—N3	175.60 (11)
C3—C2—C5—O3	−56.85 (12)	C15—N3—C16—O5	−175.86 (11)
C1—C2—C5—C17	69.79 (12)	C24—N3—C16—O5	0.88 (17)
C3—C2—C5—C17	−175.99 (9)	C15—N3—C16—C7	4.33 (17)
C5—O3—C6—C7	−20.84 (16)	C24—N3—C16—C7	−178.94 (11)
C5—O3—C6—N2	159.53 (9)	C6—C7—C16—O5	−179.37 (12)
C15—N2—C6—O3	177.01 (10)	C3—C7—C16—O5	5.85 (18)
C23—N2—C6—O3	8.66 (15)	C6—C7—C16—N3	0.43 (16)
C15—N2—C6—C7	−2.63 (17)	C3—C7—C16—N3	−174.34 (10)
C23—N2—C6—C7	−170.98 (11)	O3—C5—C17—C18	134.80 (10)
O3—C6—C7—C16	179.22 (11)	C2—C5—C17—C18	−104.13 (12)
N2—C6—C7—C16	−1.18 (17)	O3—C5—C17—C22	−48.98 (13)
O3—C6—C7—C3	−6.20 (18)	C2—C5—C17—C22	72.08 (13)
N2—C6—C7—C3	173.40 (10)	C22—C17—C18—C19	−0.94 (17)
C2—C3—C7—C6	−0.62 (15)	C5—C17—C18—C19	175.32 (11)
C4—C3—C7—C6	120.01 (12)	C17—C18—C19—C20	0.26 (18)
C2—C3—C7—C16	173.97 (10)	C18—C19—C20—C21	0.93 (18)
C4—C3—C7—C16	−65.40 (13)	C19—C20—C21—C22	−1.44 (18)
O1—S1—C8—C13	−22.94 (11)	C20—C21—C22—C17	0.76 (17)
O2—S1—C8—C13	−154.08 (9)	C18—C17—C22—C21	0.43 (17)
N1—S1—C8—C13	91.63 (10)	C5—C17—C22—C21	−175.81 (10)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10···O1^{i}	0.93	2.46	3.1846 (14)	134
C18—H18···O4^{ii}	0.93	2.47	3.2248 (15)	138
C20—H20···Cg1^{iii}	0.93	2.77	3.6038 (13)	149

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

Fig. 1

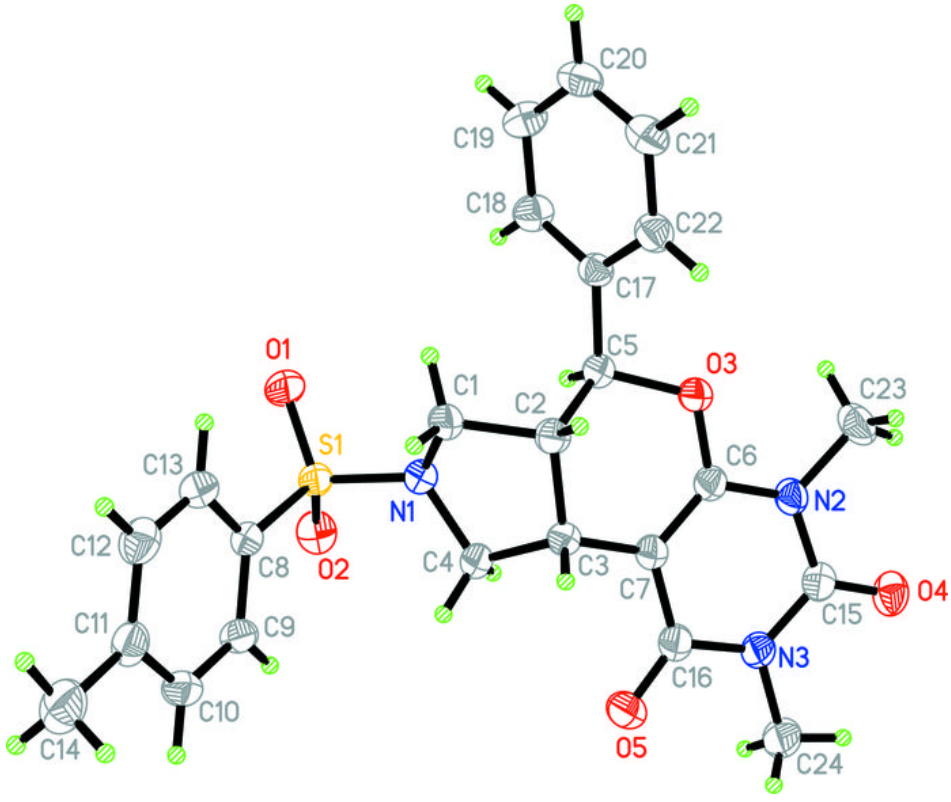
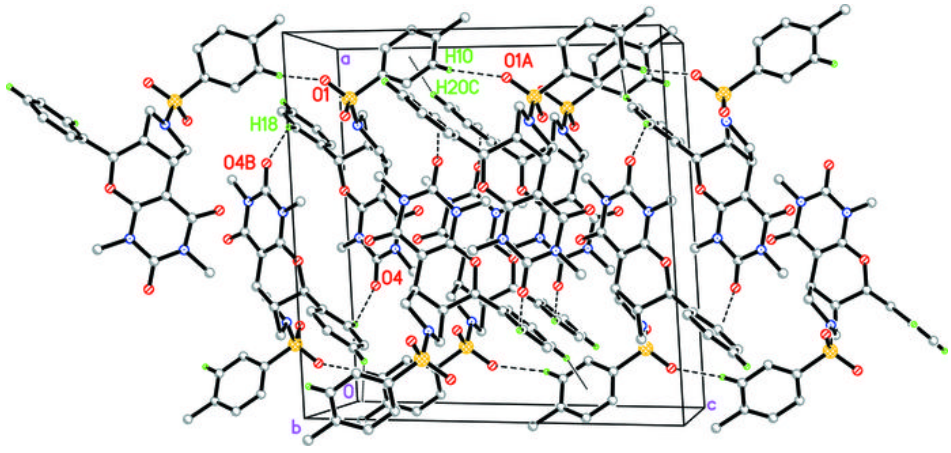

C20
C19
C21
C18
C22
C17
O1
C5
O3
C1
C2
C23
S1
C13
C6
N2
N1
C12
C8
O2
C4
C3
C7
O4
C15
C11
C9
N3
C16
C10
O5
C14
C24

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.

References

Chinnakali, K., Jayagopi, M., Sudha, D., Raghunathan, R. & Fun, H.-K. (2007*a*). *Acta Cryst.* E**63**, o4363.
Chinnakali, K., Jayagopi, M., Sudha, D., Raghunathan, R. & Fun, H.-K. (2007*b*). *Acta Cryst.* E**63**, o4364.
Chinnakali, K., Sudha, D., Jayagopi, M., Raghunathan, R. & Fun, H.-K. (2007*a*). *Acta Cryst.* E**63**, o4434–o4435.
Chinnakali, K., Sudha, D., Jayagopi, M., Raghunathan, R. & Fun, H.-K. (2007*b*). *Acta Cryst.* E**63**, o4436–o4437.
Chinnakali, K., Sudha, D., Jayagopi, M., Raghunathan, R. & Fun, H.-K. (2007*c*). *Acta Cryst.* E**63**, o4438.
Chinnakali, K., Sudha, D., Jayagopi, M., Raghunathan, R. & Fun, H.-K. (2007*d*). *Acta Cryst.* E**63**, o4489–o4490.
Chinnakali, K., Sudha, D., Jayagopi, M., Raghunathan, R. & Fun, H.-K. (2007*e*). *Acta Cryst.* E**63**, o4491–o4492.

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