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1-Ethyl-4,4,6,8-tetramethyl-2-tosyl-2,3,3a,4,6,7,8,9-octahydro-1*H*-pyrrolo[3,4-*c*]pyrano[6,5-*d*]pyrimidine-7,9-dione

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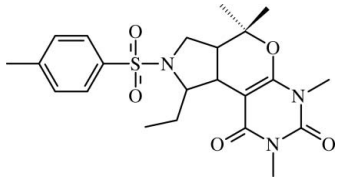
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.065; wR factor = 0.166; data-to-parameter ratio = 19.9.

The asymmetric unit of the title compound, $C_{22}H_{29}N_3O_5S$, contains two independent molecules, *A* and *B*, which differ slightly in the orientation of the ethyl and tosyl groups with respect to the attached pyrrolidine ring, as evidenced by the relevant torsion angles. In both molecules, the pyrrolidine and dihydropyran rings adopt envelope conformations, and are *trans*-fused. In molecule *A*, the tosyl group is equatorially attached to the pyrrolidine ring, whereas in *B* it is in a biaxial position. The pyrrolidine N atom exhibits sp^2 hybridization in molecule *A* and sp^3 hybridization in molecule *B*. In both molecules, the sulfonyl group has a distorted tetrahedral geometry. In the crystal structure, the molecules are linked into a three-dimensional framework by C—H···O hydrogen bonds.

Related literature

For related pyranopyrimidine structures, see: Chinnakali *et al.* (2007*a*,*b*). 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).



Experimental

Crystal data

$C_{22}H_{29}N_3O_5S$
M_r = 447.55
Triclinic, $P\overline{1}$
a = 11.6929 (3) Å
b = 11.7844 (3) Å
c = 17.9339 (4) Å
α = 71.576 (2)°
β = 88.034 (2)°
γ = 68.674 (2)°
V = 2174.87 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.19 mm^{-1}
T = 100.0 (1) K
0.35 × 0.26 × 0.23 mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.937, T_{max} = 0.958
45861 measured reflections
11377 independent reflections
7677 reflections with $I > 2\sigma(I)$
R_{int} = 0.073

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.166
S = 1.02
11377 reflections
571 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.65 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

Table 1
Selected bond and torsion angles (°).

O2*A*—S1*A*—O1*A*	119.32 (12)	O2*B*—S1*B*—O1*B*	119.55 (11)
N1*A*—S1*A*—C8*A*	105.92 (12)	N1*B*—S1*B*—C8*B*	104.49 (11)
O1*A*—S1*A*—N1*A*—C1*A*	−24.8 (2)	O1*B*—S1*B*—N1*B*—C1*B*	−11.57 (19)
C8*A*—S1*A*—N1*A*—C1*A*	88.9 (2)	C8*B*—S1*B*—N1*B*—C1*B*	102.36 (17)
N1*A*—S1*A*—C8*A*—C9*A*	107.1 (2)	N1*B*—S1*B*—C8*B*—C9*B*	112.4 (2)
N1*A*—C4*A*—C21*A*—C22*A*	56.7 (3)	N1*B*—C4*B*—C21*B*—C22*B*	−67.7 (3)

Table 2
Hydrogen-bond geometry (Å, °).

*Cg*1 is the centroid of the N2*B*/C6*B*/C7*B*/C18*B*/N3*B*/C17*B* ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1*A*—H1*B*···O4*B*^{i}	0.97	2.46	3.424 (3)	171
C1*B*—H1*C*···O1*B*	0.97	2.36	2.838 (3)	110
C1*B*—H1*D*···O4*A*^{ii}	0.97	2.40	3.346 (3)	166
C10*B*—H10*B*···O5*A*^{iii}	0.93	2.46	3.374 (3)	168
C15*A*—H15*A*···O2*A*^{iv}	0.96	2.54	3.426 (3)	153
C15*B*—H15*E*···O2*B*^{iii}	0.96	2.55	3.434 (3)	154
C16*A*—H16*C*···O4*B*^{i}	0.96	2.58	3.512 (3)	164
C20*B*—H20*E*···O4*A*^{v}	0.96	2.55	3.387 (3)	145
C21*A*—H21*A*···O5*A*	0.97	2.27	3.040 (3)	136
C21*B*—H21*D*···O5*B*	0.97	2.50	3.152 (3)	125
C21*B*—H21*D*···*Cg*1^{vi}	0.97	2.96	3.591 (3)	123

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

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* (Sheldrick, 1998); 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: WN2209).

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supplementary materials

Acta Cryst. (2007). E**63**, o4434-o4435 [**doi:10.1107/S160053680705221X**]

1-Ethyl-4,4,6,8-tetramethyl-2-tosyl-2,3,3a,4,6,7,8,9-octahydro-1*H*-pyrrolo[3,4-*c*]pyrano[6,5-*d*]pyrimidine-7,9-dione

K. Chinnakali, D. Sudha, M. Jayagopi, 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). Previously, we have reported the crystal structures of two pyrano[2,3-*d*]pyrimidine derivatives (Chinnakali *et al.*, 2007*a*,b). Now we report here the crystal structure of the title compound.

There are two independent molecules, *A* and *B*, in the asymmetric unit, with very similar conformations (Fig. 1). A superposition of the non-H atoms of molecules *A* and *B* (Fig. 2) using *XP* in *SHELXTL* (Sheldrick, 1998), gave an r.m.s. deviation of 0.437 Å. Molecules *A* and *B* differ slightly in the orientation of the ethyl and tosyl groups with respect to the attached pyrrolidine ring, as can be seen from the torsion angles given in Table 1. The geometric parameters in *A* and *B* are similar, except for some differences in the C3—C4 [1.552 (4) and 1.539 (3) Å] and C21—C22 [1.494 (4) and 1.518 (3) Å] bond lengths, and C1—N1—C4 [112.5 (2) and 109.5 (2)°] and C3—C4—C21 [117.3 (2) and 111.6 (2)°] bond angles.

In both molecules the pyrrolidine ring adopts an envelope conformation, with the local mirror plane passing through C2 and the midpoint of the bond N1—C4. The relevant asymmetry parameters (Duax *et al.*, 1976) are ΔC_S[C2] = 4.3 (2)° for molecule *A* and 9.6 (2)° for molecule *B*; Cremer & Pople puckering parameters Q and φ (Cremer & Pople, 1975) are 0.451 (3) Å and 77.2 (3)° for molecule *A*, and 0.434 (3) Å and 62.7 (3)° for molecule *B*. In both molecules, the dihydropyran ring also adopts an envelope conformation, with the local mirror plane passing through atoms C2 and C6. The asymmetry parameter ΔC_S[C2] is 5.1 (3)° for molecule *A* and 1.5 (2)° for molecule *B*; the puckering parameters Q, θ and φ are 0.507 (3) Å, 126.6 (2)° and 294.3 (3)° for molecule *A*, and 0.524 (3) Å, 126.6 (2)° and 301.6 (3)° for molecule *B*. The tosyl group is equatorially attached to the pyrrolidine ring in molecule *A* and in molecule *B* it is in a biaxial position. The sum of the bond angles around atom N1 of molecule *A* is 356.7°, indicating sp^2 hybridization, whereas in molecule *B* the corresponding value of 349.2° indicates sp^3 hybridization. In both molecules, the sulfonyl group has a distorted tetrahedral geometry (Table 1).

The C1/C3/C4/N1 plane forms dihedral angles of 33.9 (1) and 56.9 (1)°, respectively, with the O3/C5/C3/C7/C6 and C8—C13 planes in molecule *A*, and 33.2 (1) and 43.1 (1)°, respectively, in molecule *B*. The dihedral angle between the O3/C5/C3/C7/C6 and C7/C6/N2/C17/N3/C18 planes is 2.6 (1)° in *A* and 0.7 (1)° in *B*. The pyrrolidine ring in both molecules is *trans*-fused to the dihydropyran ring.

Each of the independent molecules exists as a C—H···O hydrogen-bonded dimer, generating a ring of graph-set motif $R^2_2(16)$. The C1A—H1B···O4B^{i} and C16A—H16C···O4B^{i} hydrogen bonding interactions (Table 2) form a pair of bifurcated acceptor bonds, generating a ring of graph-set motif $R^1_2(7)$. The above two interactions along with the C1B—H1D···O4A^{ii} interaction link molecules *A* and *B* into a chain along the [111] direction. The dimers and the chains are cross-linked into a three-dimensional network by C10B—H10B···O5A^{iii} and C20B—H20E···O4A^{v} hydrogen bonding interactions, and C—H···π interactions involving the N2B/C6B/C7B/C18B/N3B/C17B ring (centroid *Cg*1). The geometry of the hydrogen

bonds and symmetry codes are given in Table 2. A short H20D···H22C(−1 + *x*,1 + *y*,*z*) contact of 2.06 Å is observed in the crystal structure.

Experimental

To a solution of 1,3-dimethylpyrimidine-2,4,6-trione (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

All 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.

Figures

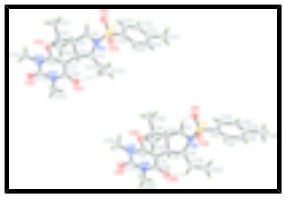


Fig. 1. The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 80% probability level. Hydrogen bonds are shown as dashed lines.

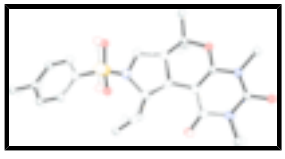


Fig. 2. Fit of molecule A (dashed lines) on molecule B (solid lines). H atoms have been omitted for clarity.

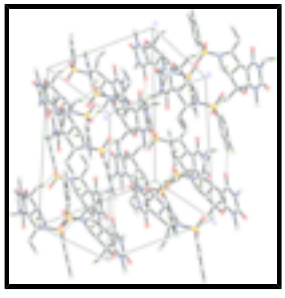


Fig. 3. View of the crystal packing of the title compound. Hydrogen bonds are shown as dashed lines. For the sake of clarity, H atoms not involved in the interactions have been omitted.

1-Ethyl-4,4,6,8-tetramethyl-2-tosyl-2,3,3a,4,6,7,8,9-octahydro-1*H*-\ pyrrolo[3,4-*c*]pyrano[6,5-*d*]pyrimidine-7,9-dione

Crystal data

$C_{22}H_{29}N_3O_5S$	$Z = 4$
$M_r = 447.55$	$F_{000} = 952$

Triclinic, $P\bar{1}$	D_x = 1.367 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 11.6929 (3) Å	Cell parameters from 5742 reflections
b = 11.7844 (3) Å	θ = 2.3–29.5º
c = 17.9339 (4) Å	μ = 0.19 mm^{-1}
α = 71.576 (2)º	T = 100.0 (1) K
β = 88.034 (2)º	Block, brown
γ = 68.674 (2)º	0.35 × 0.26 × 0.23 mm
V = 2174.87 (10) Å^3	

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer	11377 independent reflections
Radiation source: fine-focus sealed tube	7677 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.073
Detector resolution: 8.33 pixels mm^{-1}	θ_{max} = 29.0º
T = 100.0(1) K	θ_{min} = 1.2º
ω scans	h = −15→15
Absorption correction: multi-scan (SADABS; Bruker, 2005)	k = −15→16
T_{min} = 0.937, T_{max} = 0.958	l = −24→24
45861 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
$R[F^2 > 2\sigma(F^2)]$ = 0.065	H-atom parameters constrained
$wR(F^2)$ = 0.166	$w = 1/[\sigma^2(F_o^2) + (0.0718P)^2 + 1.2173P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max}$ = 0.001
11377 reflections	$\Delta\rho_{max}$ = 0.65 e Å^{-3}
571 parameters	$\Delta\rho_{min}$ = −0.53 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}
S1A	0.48868 (6)	−0.06781 (6)	0.18394 (4)	0.02654 (16)
O1A	0.56474 (17)	−0.18205 (18)	0.16642 (11)	0.0320 (4)
O2A	0.35726 (16)	−0.02178 (19)	0.16876 (11)	0.0356 (5)
O3A	0.68594 (14)	0.23695 (16)	−0.09004 (9)	0.0242 (4)
O4A	0.38858 (16)	0.55931 (16)	−0.26961 (10)	0.0269 (4)
O5A	0.29679 (16)	0.46092 (17)	−0.01454 (10)	0.0324 (4)
N1A	0.53278 (19)	0.0476 (2)	0.13825 (12)	0.0283 (5)
N2A	0.53767 (18)	0.40242 (19)	−0.17589 (11)	0.0227 (4)
N3A	0.34189 (17)	0.50835 (18)	−0.14220 (11)	0.0212 (4)
C1A	0.6604 (2)	0.0218 (2)	0.11508 (14)	0.0245 (5)
H1A	0.7011	−0.0665	0.1159	0.029*
H1B	0.7095	0.0407	0.1485	0.029*
C2A	0.6343 (2)	0.1162 (2)	0.03180 (13)	0.0212 (5)
H2A	0.5965	0.0835	−0.0004	0.025*
C3A	0.5341 (2)	0.2365 (2)	0.04071 (13)	0.0219 (5)
H3A	0.5706	0.2728	0.0712	0.026*
C4A	0.4443 (2)	0.1815 (2)	0.09144 (14)	0.0264 (5)
H4A	0.3861	0.1744	0.0568	0.032*
C5A	0.7400 (2)	0.1437 (2)	−0.01069 (13)	0.0217 (5)
C6A	0.5700 (2)	0.3222 (2)	−0.09877 (13)	0.0209 (5)
C7A	0.4910 (2)	0.3325 (2)	−0.04139 (13)	0.0212 (5)
C8A	0.5229 (2)	−0.1002 (2)	0.28523 (14)	0.0235 (5)
C9A	0.4279 (2)	−0.0639 (2)	0.33189 (15)	0.0265 (5)
H9A	0.3466	−0.0221	0.3098	0.032*
C10A	0.4554 (2)	−0.0906 (2)	0.41181 (15)	0.0267 (5)
H10A	0.3919	−0.0652	0.4428	0.032*
C11A	0.5759 (2)	−0.1544 (2)	0.44643 (14)	0.0257 (5)
C12A	0.6702 (2)	−0.1893 (2)	0.39848 (14)	0.0252 (5)
H12A	0.7515	−0.2312	0.4206	0.030*
C13A	0.6447 (2)	−0.1624 (2)	0.31842 (14)	0.0238 (5)
H13A	0.7084	−0.1857	0.2871	0.029*
C14A	0.6040 (3)	−0.1857 (3)	0.53346 (15)	0.0364 (7)
H14A	0.5364	−0.1313	0.5534	0.055*
H14B	0.6776	−0.1715	0.5421	0.055*
H14C	0.6161	−0.2743	0.5603	0.055*
C15A	0.8300 (2)	0.0273 (2)	−0.02821 (15)	0.0287 (6)
H15A	0.7862	−0.0047	−0.0557	0.043*
H15B	0.8707	−0.0387	0.0204	0.043*
H15C	0.8901	0.0513	−0.0604	0.043*
C16A	0.8046 (2)	0.2045 (3)	0.02814 (15)	0.0289 (6)

H16A	0.7479	0.2877	0.0275	0.043*
H16B	0.8735	0.2138	−0.0003	0.043*
H16C	0.8332	0.1504	0.0817	0.043*
C17A	0.4200 (2)	0.4935 (2)	−0.20027 (13)	0.0208 (5)
C18A	0.3723 (2)	0.4348 (2)	−0.06183 (14)	0.0222 (5)
C19A	0.6236 (2)	0.3851 (3)	−0.23633 (15)	0.0331 (6)
H19A	0.7045	0.3699	−0.2158	0.050*
H19B	0.5969	0.4613	−0.2819	0.050*
H19C	0.6258	0.3127	−0.2509	0.050*
C20A	0.2178 (2)	0.6067 (2)	−0.16769 (15)	0.0280 (6)
H20A	0.1843	0.5975	−0.2126	0.042*
H20B	0.2218	0.6908	−0.1818	0.042*
H20C	0.1659	0.5964	−0.1254	0.042*
C21A	0.3727 (2)	0.2528 (3)	0.14626 (15)	0.0298 (6)
H21A	0.3189	0.3385	0.1142	0.036*
H21B	0.3207	0.2082	0.1741	0.036*
C22A	0.4492 (3)	0.2658 (3)	0.2058 (2)	0.0517 (9)
H22A	0.3968	0.3026	0.2412	0.078*
H22B	0.4920	0.3208	0.1793	0.078*
H22C	0.5079	0.1823	0.2351	0.078*
S1B	−0.01441 (5)	0.47939 (6)	0.68320 (3)	0.02278 (15)
O1B	0.04714 (17)	0.37022 (16)	0.65714 (10)	0.0286 (4)
O2B	−0.14485 (15)	0.54805 (17)	0.66426 (10)	0.0282 (4)
O3B	0.17436 (15)	0.72899 (16)	0.40075 (9)	0.0251 (4)
O4B	−0.13875 (17)	1.05506 (17)	0.23361 (10)	0.0313 (4)
O5B	−0.18272 (15)	0.97693 (16)	0.49596 (10)	0.0269 (4)
N1B	0.05370 (17)	0.58236 (18)	0.65284 (11)	0.0215 (4)
N2B	0.01738 (19)	0.89330 (19)	0.32009 (11)	0.0251 (5)
N3B	−0.16202 (18)	1.01317 (18)	0.36477 (11)	0.0217 (4)
C1B	0.1748 (2)	0.5421 (2)	0.61971 (13)	0.0220 (5)
H1C	0.2060	0.4511	0.6256	0.026*
H1D	0.2355	0.5608	0.6441	0.026*
C2B	0.1399 (2)	0.6257 (2)	0.53363 (13)	0.0188 (5)
H2B	0.0877	0.5942	0.5105	0.023*
C3B	0.0581 (2)	0.7557 (2)	0.54064 (13)	0.0192 (5)
H3B	0.1116	0.7928	0.5570	0.023*
C4B	−0.0202 (2)	0.7234 (2)	0.60906 (13)	0.0211 (5)
H4B	−0.1013	0.7341	0.5885	0.025*
C5B	0.2395 (2)	0.6380 (2)	0.47907 (13)	0.0217 (5)
C6B	0.0629 (2)	0.8193 (2)	0.39714 (14)	0.0219 (5)
C7B	−0.0016 (2)	0.8415 (2)	0.45937 (13)	0.0198 (5)
C8B	0.0138 (2)	0.4238 (2)	0.78687 (14)	0.0212 (5)
C9B	−0.0840 (2)	0.4554 (2)	0.83259 (14)	0.0239 (5)
H9B	−0.1638	0.5033	0.8088	0.029*
C10B	−0.0613 (2)	0.4149 (2)	0.91380 (14)	0.0249 (5)
H10B	−0.1267	0.4362	0.9443	0.030*
C11B	0.0579 (2)	0.3427 (2)	0.95091 (14)	0.0235 (5)
C12B	0.1548 (2)	0.3116 (2)	0.90366 (14)	0.0223 (5)
H12B	0.2347	0.2630	0.9273	0.027*

C13B	0.1334 (2)	0.3519 (2)	0.82234 (14)	0.0233 (5)
H13B	0.1986	0.3312	0.7916	0.028*
C14B	0.0812 (3)	0.3002 (3)	1.03904 (15)	0.0304 (6)
H14D	0.0449	0.2377	1.0629	0.046*
H14F	0.0452	0.3733	1.0569	0.046*
H14E	0.1684	0.2624	1.0537	0.046*
C15B	0.3098 (2)	0.5137 (2)	0.46255 (14)	0.0266 (5)
H15D	0.3662	0.5277	0.4237	0.040*
H15E	0.2529	0.4857	0.4431	0.040*
H15F	0.3550	0.4488	0.5104	0.040*
C16B	0.3255 (2)	0.6925 (2)	0.50306 (16)	0.0286 (6)
H16D	0.2796	0.7789	0.5025	0.043*
H16E	0.3877	0.6931	0.4667	0.043*
H16F	0.3641	0.6401	0.5553	0.043*
C17B	−0.0974 (2)	0.9910 (2)	0.30195 (14)	0.0233 (5)
C18B	−0.1188 (2)	0.9448 (2)	0.44484 (13)	0.0209 (5)
C19B	0.0888 (3)	0.8655 (3)	0.25440 (14)	0.0371 (7)
H19D	0.0448	0.9268	0.2052	0.056*
H19E	0.1005	0.7801	0.2553	0.056*
H19F	0.1675	0.8716	0.2599	0.056*
C20B	−0.2844 (2)	1.1152 (2)	0.34687 (15)	0.0286 (6)
H20D	−0.3280	1.1097	0.3045	0.043*
H20E	−0.2765	1.1975	0.3315	0.043*
H20F	−0.3292	1.1053	0.3928	0.043*
C21B	−0.0342 (2)	0.8060 (2)	0.66169 (13)	0.0230 (5)
H21C	0.0471	0.7899	0.6835	0.028*
H21D	−0.0695	0.8960	0.6293	0.028*
C22B	−0.1138 (2)	0.7828 (2)	0.72915 (15)	0.0302 (6)
H22D	−0.1927	0.7921	0.7087	0.045*
H22E	−0.1249	0.8444	0.7559	0.045*
H22F	−0.0743	0.6973	0.7655	0.045*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1A	0.0270 (3)	0.0263 (3)	0.0237 (3)	−0.0093 (3)	0.0002 (2)	−0.0053 (3)
O1A	0.0379 (10)	0.0300 (10)	0.0316 (10)	−0.0135 (9)	0.0048 (8)	−0.0138 (8)
O2A	0.0280 (10)	0.0426 (12)	0.0328 (10)	−0.0134 (9)	−0.0022 (8)	−0.0070 (9)
O3A	0.0218 (8)	0.0204 (9)	0.0191 (8)	0.0009 (7)	−0.0006 (6)	−0.0017 (7)
O4A	0.0324 (10)	0.0213 (9)	0.0202 (9)	−0.0063 (7)	−0.0052 (7)	−0.0013 (7)
O5A	0.0324 (10)	0.0242 (10)	0.0248 (9)	0.0032 (8)	0.0055 (7)	−0.0038 (8)
N1A	0.0223 (10)	0.0217 (11)	0.0278 (11)	−0.0018 (9)	0.0002 (8)	0.0018 (9)
N2A	0.0245 (10)	0.0180 (10)	0.0186 (10)	−0.0023 (8)	−0.0003 (8)	−0.0032 (8)
N3A	0.0220 (10)	0.0141 (9)	0.0209 (10)	−0.0018 (8)	−0.0018 (8)	−0.0023 (8)
C1A	0.0225 (12)	0.0193 (12)	0.0233 (12)	−0.0026 (10)	−0.0008 (9)	−0.0014 (10)
C2A	0.0212 (11)	0.0156 (11)	0.0215 (12)	−0.0032 (9)	−0.0028 (9)	−0.0028 (9)
C3A	0.0250 (12)	0.0170 (11)	0.0179 (11)	−0.0023 (9)	−0.0018 (9)	−0.0042 (9)
C4A	0.0258 (12)	0.0226 (13)	0.0215 (12)	−0.0034 (10)	−0.0043 (9)	−0.0007 (10)

C5A	0.0229 (12)	0.0175 (11)	0.0173 (11)	−0.0039 (9)	−0.0047 (9)	0.0007 (9)
C6A	0.0219 (11)	0.0160 (11)	0.0204 (11)	−0.0031 (9)	−0.0024 (9)	−0.0043 (9)
C7A	0.0235 (12)	0.0155 (11)	0.0193 (11)	−0.0025 (9)	−0.0025 (9)	−0.0038 (9)
C8A	0.0283 (13)	0.0164 (11)	0.0241 (12)	−0.0090 (10)	0.0030 (9)	−0.0037 (10)
C9A	0.0269 (13)	0.0173 (12)	0.0319 (14)	−0.0073 (10)	0.0032 (10)	−0.0045 (10)
C10A	0.0318 (13)	0.0150 (11)	0.0310 (14)	−0.0076 (10)	0.0091 (10)	−0.0063 (10)
C11A	0.0352 (14)	0.0143 (11)	0.0267 (13)	−0.0081 (10)	0.0036 (10)	−0.0071 (10)
C12A	0.0284 (13)	0.0152 (11)	0.0284 (13)	−0.0054 (10)	−0.0005 (10)	−0.0050 (10)
C13A	0.0260 (12)	0.0159 (11)	0.0273 (13)	−0.0061 (10)	0.0043 (10)	−0.0064 (10)
C14A	0.0501 (17)	0.0266 (14)	0.0269 (14)	−0.0072 (13)	0.0023 (12)	−0.0094 (12)
C15A	0.0233 (12)	0.0246 (13)	0.0271 (13)	0.0005 (10)	0.0002 (10)	−0.0048 (11)
C16A	0.0302 (13)	0.0251 (13)	0.0273 (13)	−0.0115 (11)	−0.0041 (10)	−0.0013 (11)
C17A	0.0257 (12)	0.0139 (11)	0.0206 (12)	−0.0053 (9)	−0.0030 (9)	−0.0047 (9)
C18A	0.0262 (12)	0.0137 (11)	0.0216 (12)	−0.0028 (9)	−0.0018 (9)	−0.0038 (9)
C19A	0.0309 (14)	0.0327 (15)	0.0213 (13)	−0.0013 (12)	0.0054 (10)	−0.0027 (11)
C20A	0.0272 (13)	0.0178 (12)	0.0264 (13)	0.0013 (10)	−0.0033 (10)	−0.0013 (10)
C21A	0.0314 (14)	0.0270 (14)	0.0244 (13)	−0.0061 (11)	0.0020 (10)	−0.0054 (11)
C22A	0.0455 (19)	0.057 (2)	0.061 (2)	−0.0115 (16)	−0.0033 (15)	−0.0380 (18)
S1B	0.0253 (3)	0.0189 (3)	0.0208 (3)	−0.0067 (2)	−0.0011 (2)	−0.0036 (2)
O1B	0.0377 (10)	0.0221 (9)	0.0284 (9)	−0.0124 (8)	0.0025 (8)	−0.0097 (8)
O2B	0.0248 (9)	0.0265 (10)	0.0291 (10)	−0.0091 (8)	−0.0032 (7)	−0.0036 (8)
O3B	0.0262 (9)	0.0185 (8)	0.0197 (8)	0.0009 (7)	0.0021 (7)	−0.0027 (7)
O4B	0.0396 (11)	0.0227 (9)	0.0205 (9)	−0.0025 (8)	−0.0090 (7)	−0.0021 (7)
O5B	0.0276 (9)	0.0199 (9)	0.0241 (9)	−0.0003 (7)	0.0023 (7)	−0.0053 (7)
N1B	0.0212 (10)	0.0139 (9)	0.0207 (10)	−0.0017 (8)	−0.0003 (7)	0.0002 (8)
N2B	0.0311 (11)	0.0188 (10)	0.0164 (10)	−0.0012 (9)	−0.0002 (8)	−0.0031 (8)
N3B	0.0238 (10)	0.0141 (9)	0.0207 (10)	−0.0023 (8)	−0.0034 (8)	−0.0020 (8)
C1B	0.0212 (11)	0.0164 (11)	0.0219 (12)	−0.0024 (9)	0.0004 (9)	−0.0029 (9)
C2B	0.0181 (11)	0.0141 (11)	0.0199 (11)	−0.0022 (9)	−0.0013 (8)	−0.0040 (9)
C3B	0.0218 (11)	0.0142 (11)	0.0172 (11)	−0.0027 (9)	−0.0005 (8)	−0.0037 (9)
C4B	0.0240 (12)	0.0125 (11)	0.0188 (11)	−0.0015 (9)	−0.0016 (9)	−0.0002 (9)
C5B	0.0231 (12)	0.0141 (11)	0.0189 (11)	0.0003 (9)	−0.0039 (9)	−0.0014 (9)
C6B	0.0245 (12)	0.0157 (11)	0.0205 (12)	−0.0037 (9)	−0.0011 (9)	−0.0035 (9)
C7B	0.0232 (11)	0.0133 (11)	0.0190 (11)	−0.0035 (9)	−0.0030 (9)	−0.0035 (9)
C8B	0.0270 (12)	0.0118 (11)	0.0210 (12)	−0.0057 (9)	−0.0002 (9)	−0.0018 (9)
C9B	0.0233 (12)	0.0163 (11)	0.0262 (13)	−0.0053 (10)	0.0006 (9)	−0.0014 (10)
C10B	0.0290 (13)	0.0168 (12)	0.0271 (13)	−0.0078 (10)	0.0077 (10)	−0.0060 (10)
C11B	0.0296 (13)	0.0170 (11)	0.0234 (12)	−0.0084 (10)	0.0024 (10)	−0.0064 (10)
C12B	0.0234 (12)	0.0167 (11)	0.0232 (12)	−0.0049 (9)	−0.0003 (9)	−0.0046 (10)
C13B	0.0263 (12)	0.0168 (12)	0.0225 (12)	−0.0050 (10)	0.0042 (9)	−0.0044 (10)
C14B	0.0385 (15)	0.0261 (14)	0.0254 (13)	−0.0106 (12)	0.0036 (11)	−0.0085 (11)
C15B	0.0262 (12)	0.0208 (12)	0.0255 (13)	−0.0010 (10)	0.0018 (10)	−0.0070 (10)
C16B	0.0273 (13)	0.0230 (13)	0.0336 (14)	−0.0093 (11)	0.0034 (10)	−0.0066 (11)
C17B	0.0287 (13)	0.0175 (12)	0.0216 (12)	−0.0063 (10)	−0.0034 (9)	−0.0057 (10)
C18B	0.0230 (12)	0.0141 (11)	0.0213 (12)	−0.0041 (9)	−0.0021 (9)	−0.0028 (9)
C19B	0.0424 (16)	0.0354 (16)	0.0170 (12)	0.0008 (13)	0.0038 (11)	−0.0049 (11)
C20B	0.0254 (13)	0.0211 (13)	0.0264 (13)	0.0015 (10)	−0.0071 (10)	−0.0017 (10)
C21B	0.0288 (12)	0.0161 (11)	0.0184 (11)	−0.0040 (10)	−0.0010 (9)	−0.0030 (9)
C22B	0.0373 (15)	0.0241 (13)	0.0251 (13)	−0.0061 (11)	0.0062 (11)	−0.0091 (11)

Geometric parameters (Å, °)

S1A—O2A	1.4349 (19)	S1B—O2B	1.4356 (17)
S1A—O1A	1.4421 (18)	S1B—O1B	1.4405 (17)
S1A—N1A	1.602 (2)	S1B—N1B	1.630 (2)
S1A—C8A	1.762 (2)	S1B—C8B	1.763 (2)
O3A—C6A	1.340 (3)	O3B—C6B	1.337 (3)
O3A—C5A	1.483 (3)	O3B—C5B	1.493 (3)
O4A—C17A	1.224 (3)	O4B—C17B	1.223 (3)
O5A—C18A	1.229 (3)	O5B—C18B	1.229 (3)
N1A—C1A	1.483 (3)	N1B—C1B	1.488 (3)
N1A—C4A	1.516 (3)	N1B—C4B	1.518 (3)
N2A—C6A	1.378 (3)	N2B—C17B	1.379 (3)
N2A—C17A	1.381 (3)	N2B—C6B	1.380 (3)
N2A—C19A	1.464 (3)	N2B—C19B	1.473 (3)
N3A—C17A	1.372 (3)	N3B—C17B	1.376 (3)
N3A—C18A	1.406 (3)	N3B—C18B	1.410 (3)
N3A—C20A	1.465 (3)	N3B—C20B	1.460 (3)
C1A—C2A	1.515 (3)	C1B—C2B	1.520 (3)
C1A—H1A	0.97	C1B—H1C	0.97
C1A—H1B	0.97	C1B—H1D	0.97
C2A—C5A	1.511 (3)	C2B—C5B	1.513 (3)
C2A—C3A	1.526 (3)	C2B—C3B	1.525 (3)
C2A—H2A	0.98	C2B—H2B	0.98
C3A—C7A	1.512 (3)	C3B—C7B	1.503 (3)
C3A—C4A	1.552 (4)	C3B—C4B	1.539 (3)
C3A—H3A	0.98	C3B—H3B	0.98
C4A—C21A	1.526 (3)	C4B—C21B	1.523 (3)
C4A—H4A	0.98	C4B—H4B	0.98
C5A—C15A	1.513 (3)	C5B—C16B	1.512 (4)
C5A—C16A	1.521 (3)	C5B—C15B	1.513 (3)
C6A—C7A	1.363 (3)	C6B—C7B	1.366 (3)
C7A—C18A	1.433 (3)	C7B—C18B	1.428 (3)
C8A—C9A	1.391 (3)	C8B—C9B	1.391 (3)
C8A—C13A	1.394 (3)	C8B—C13B	1.392 (3)
C9A—C10A	1.389 (3)	C9B—C10B	1.384 (3)
C9A—H9A	0.93	C9B—H9B	0.93
C10A—C11A	1.389 (3)	C10B—C11B	1.397 (3)
C10A—H10A	0.93	C10B—H10B	0.93
C11A—C12A	1.398 (3)	C11B—C12B	1.402 (3)
C11A—C14A	1.504 (3)	C11B—C14B	1.501 (3)
C12A—C13A	1.387 (3)	C12B—C13B	1.384 (3)
C12A—H12A	0.93	C12B—H12B	0.93
C13A—H13A	0.93	C13B—H13B	0.93
C14A—H14A	0.96	C14B—H14D	0.96
C14A—H14B	0.96	C14B—H14F	0.96
C14A—H14C	0.96	C14B—H14E	0.96
C15A—H15A	0.96	C15B—H15D	0.96

C15A—H15B	0.96	C15B—H15E	0.96
C15A—H15C	0.96	C15B—H15F	0.96
C16A—H16A	0.96	C16B—H16D	0.96
C16A—H16B	0.96	C16B—H16E	0.96
C16A—H16C	0.96	C16B—H16F	0.96
C19A—H19A	0.96	C19B—H19D	0.96
C19A—H19B	0.96	C19B—H19E	0.96
C19A—H19C	0.96	C19B—H19F	0.96
C20A—H20A	0.96	C20B—H20D	0.96
C20A—H20B	0.96	C20B—H20E	0.96
C20A—H20C	0.96	C20B—H20F	0.96
C21A—C22A	1.494 (4)	C21B—C22B	1.518 (3)
C21A—H21A	0.97	C21B—H21C	0.97
C21A—H21B	0.97	C21B—H21D	0.97
C22A—H22A	0.96	C22B—H22D	0.96
C22A—H22B	0.96	C22B—H22E	0.96
C22A—H22C	0.96	C22B—H22F	0.96
O2A—S1A—O1A	119.32 (12)	O2B—S1B—O1B	119.55 (11)
O2A—S1A—N1A	107.97 (11)	O2B—S1B—N1B	108.35 (10)
O1A—S1A—N1A	108.82 (11)	O1B—S1B—N1B	109.20 (11)
O2A—S1A—C8A	107.96 (11)	O2B—S1B—C8B	107.46 (11)
O1A—S1A—C8A	106.09 (11)	O1B—S1B—C8B	106.77 (11)
N1A—S1A—C8A	105.92 (12)	N1B—S1B—C8B	104.49 (11)
C6A—O3A—C5A	119.34 (17)	C6B—O3B—C5B	119.78 (17)
C1A—N1A—C4A	112.5 (2)	C1B—N1B—C4B	109.53 (18)
C1A—N1A—S1A	121.13 (16)	C1B—N1B—S1B	118.94 (15)
C4A—N1A—S1A	123.19 (17)	C4B—N1B—S1B	120.74 (16)
C6A—N2A—C17A	121.34 (19)	C17B—N2B—C6B	121.58 (19)
C6A—N2A—C19A	120.77 (19)	C17B—N2B—C19B	118.04 (19)
C17A—N2A—C19A	117.62 (19)	C6B—N2B—C19B	120.32 (19)
C17A—N3A—C18A	124.64 (19)	C17B—N3B—C18B	124.85 (19)
C17A—N3A—C20A	116.39 (19)	C17B—N3B—C20B	117.32 (19)
C18A—N3A—C20A	118.95 (19)	C18B—N3B—C20B	117.83 (19)
N1A—C1A—C2A	100.01 (18)	N1B—C1B—C2B	100.96 (17)
N1A—C1A—H1A	111.8	N1B—C1B—H1C	111.6
C2A—C1A—H1A	111.8	C2B—C1B—H1C	111.6
N1A—C1A—H1B	111.8	N1B—C1B—H1D	111.6
C2A—C1A—H1B	111.8	C2B—C1B—H1D	111.6
H1A—C1A—H1B	109.5	H1C—C1B—H1D	109.4
C5A—C2A—C1A	119.02 (19)	C5B—C2B—C1B	120.04 (18)
C5A—C2A—C3A	112.9 (2)	C5B—C2B—C3B	111.6 (2)
C1A—C2A—C3A	102.73 (18)	C1B—C2B—C3B	101.85 (17)
C5A—C2A—H2A	107.2	C5B—C2B—H2B	107.6
C1A—C2A—H2A	107.2	C1B—C2B—H2B	107.6
C3A—C2A—H2A	107.2	C3B—C2B—H2B	107.6
C7A—C3A—C2A	106.90 (18)	C7B—C3B—C2B	107.04 (17)
C7A—C3A—C4A	120.5 (2)	C7B—C3B—C4B	120.97 (19)
C2A—C3A—C4A	102.81 (19)	C2B—C3B—C4B	104.91 (18)
C7A—C3A—H3A	108.7	C7B—C3B—H3B	107.8

C2A—C3A—H3A	108.7	C2B—C3B—H3B	107.8
C4A—C3A—H3A	108.7	C4B—C3B—H3B	107.8
N1A—C4A—C21A	110.93 (19)	N1B—C4B—C21B	111.43 (18)
N1A—C4A—C3A	100.64 (18)	N1B—C4B—C3B	102.66 (17)
C21A—C4A—C3A	117.3 (2)	C21B—C4B—C3B	111.6 (2)
N1A—C4A—H4A	109.2	N1B—C4B—H4B	110.3
C21A—C4A—H4A	109.2	C21B—C4B—H4B	110.3
C3A—C4A—H4A	109.2	C3B—C4B—H4B	110.3
O3A—C5A—C2A	106.18 (17)	O3B—C5B—C16B	107.2 (2)
O3A—C5A—C15A	103.56 (18)	O3B—C5B—C2B	106.21 (17)
C2A—C5A—C15A	112.1 (2)	C16B—C5B—C2B	115.17 (19)
O3A—C5A—C16A	107.48 (19)	O3B—C5B—C15B	103.75 (18)
C2A—C5A—C16A	114.5 (2)	C16B—C5B—C15B	111.6 (2)
C15A—C5A—C16A	112.1 (2)	C2B—C5B—C15B	112.0 (2)
O3A—C6A—C7A	126.8 (2)	O3B—C6B—C7B	126.8 (2)
O3A—C6A—N2A	110.75 (19)	O3B—C6B—N2B	111.38 (19)
C7A—C6A—N2A	122.5 (2)	C7B—C6B—N2B	121.8 (2)
C6A—C7A—C18A	118.3 (2)	C6B—C7B—C18B	119.4 (2)
C6A—C7A—C3A	118.2 (2)	C6B—C7B—C3B	117.01 (19)
C18A—C7A—C3A	123.5 (2)	C18B—C7B—C3B	123.5 (2)
C9A—C8A—C13A	120.2 (2)	C9B—C8B—C13B	120.4 (2)
C9A—C8A—S1A	119.74 (19)	C9B—C8B—S1B	119.44 (18)
C13A—C8A—S1A	120.07 (18)	C13B—C8B—S1B	120.09 (18)
C10A—C9A—C8A	119.5 (2)	C10B—C9B—C8B	119.4 (2)
C10A—C9A—H9A	120.3	C10B—C9B—H9B	120.3
C8A—C9A—H9A	120.3	C8B—C9B—H9B	120.3
C9A—C10A—C11A	121.3 (2)	C9B—C10B—C11B	121.3 (2)
C9A—C10A—H10A	119.3	C9B—C10B—H10B	119.3
C11A—C10A—H10A	119.3	C11B—C10B—H10B	119.3
C10A—C11A—C12A	118.4 (2)	C10B—C11B—C12B	118.3 (2)
C10A—C11A—C14A	120.8 (2)	C10B—C11B—C14B	120.7 (2)
C12A—C11A—C14A	120.8 (2)	C12B—C11B—C14B	121.0 (2)
C13A—C12A—C11A	121.1 (2)	C13B—C12B—C11B	121.0 (2)
C13A—C12A—H12A	119.4	C13B—C12B—H12B	119.5
C11A—C12A—H12A	119.4	C11B—C12B—H12B	119.5
C12A—C13A—C8A	119.5 (2)	C12B—C13B—C8B	119.6 (2)
C12A—C13A—H13A	120.2	C12B—C13B—H13B	120.2
C8A—C13A—H13A	120.2	C8B—C13B—H13B	120.2
C11A—C14A—H14A	109.5	C11B—C14B—H14D	109.5
C11A—C14A—H14B	109.5	C11B—C14B—H14F	109.5
H14A—C14A—H14B	109.5	H14D—C14B—H14F	109.5
C11A—C14A—H14C	109.5	C11B—C14B—H14E	109.5
H14A—C14A—H14C	109.5	H14D—C14B—H14E	109.5
H14B—C14A—H14C	109.5	H14F—C14B—H14E	109.5
C5A—C15A—H15A	109.5	C5B—C15B—H15D	109.5
C5A—C15A—H15B	109.5	C5B—C15B—H15E	109.5
H15A—C15A—H15B	109.5	H15D—C15B—H15E	109.5
C5A—C15A—H15C	109.5	C5B—C15B—H15F	109.5
H15A—C15A—H15C	109.5	H15D—C15B—H15F	109.5

H15B—C15A—H15C	109.5	H15E—C15B—H15F	109.5
C5A—C16A—H16A	109.5	C5B—C16B—H16D	109.5
C5A—C16A—H16B	109.5	C5B—C16B—H16E	109.5
H16A—C16A—H16B	109.5	H16D—C16B—H16E	109.5
C5A—C16A—H16C	109.5	C5B—C16B—H16F	109.5
H16A—C16A—H16C	109.5	H16D—C16B—H16F	109.5
H16B—C16A—H16C	109.5	H16E—C16B—H16F	109.5
O4A—C17A—N3A	122.1 (2)	O4B—C17B—N3B	122.0 (2)
O4A—C17A—N2A	121.6 (2)	O4B—C17B—N2B	121.6 (2)
N3A—C17A—N2A	116.27 (19)	N3B—C17B—N2B	116.4 (2)
O5A—C18A—N3A	118.9 (2)	O5B—C18B—N3B	119.0 (2)
O5A—C18A—C7A	124.7 (2)	O5B—C18B—C7B	125.2 (2)
N3A—C18A—C7A	116.5 (2)	N3B—C18B—C7B	115.8 (2)
N2A—C19A—H19A	109.5	N2B—C19B—H19D	109.5
N2A—C19A—H19B	109.5	N2B—C19B—H19E	109.5
H19A—C19A—H19B	109.5	H19D—C19B—H19E	109.5
N2A—C19A—H19C	109.5	N2B—C19B—H19F	109.5
H19A—C19A—H19C	109.5	H19D—C19B—H19F	109.5
H19B—C19A—H19C	109.5	H19E—C19B—H19F	109.5
N3A—C20A—H20A	109.5	N3B—C20B—H20D	109.5
N3A—C20A—H20B	109.5	N3B—C20B—H20E	109.5
H20A—C20A—H20B	109.5	H20D—C20B—H20E	109.5
N3A—C20A—H20C	109.5	N3B—C20B—H20F	109.5
H20A—C20A—H20C	109.5	H20D—C20B—H20F	109.5
H20B—C20A—H20C	109.5	H20E—C20B—H20F	109.5
C22A—C21A—C4A	115.6 (2)	C22B—C21B—C4B	114.8 (2)
C22A—C21A—H21A	108.4	C22B—C21B—H21C	108.6
C4A—C21A—H21A	108.4	C4B—C21B—H21C	108.6
C22A—C21A—H21B	108.4	C22B—C21B—H21D	108.6
C4A—C21A—H21B	108.4	C4B—C21B—H21D	108.6
H21A—C21A—H21B	107.4	H21C—C21B—H21D	107.5
C21A—C22A—H22A	109.5	C21B—C22B—H22D	109.5
C21A—C22A—H22B	109.5	C21B—C22B—H22E	109.5
H22A—C22A—H22B	109.5	H22D—C22B—H22E	109.5
C21A—C22A—H22C	109.5	C21B—C22B—H22F	109.5
H22A—C22A—H22C	109.5	H22D—C22B—H22F	109.5
H22B—C22A—H22C	109.5	H22E—C22B—H22F	109.5
O2A—S1A—N1A—C1A	−155.63 (19)	O2B—S1B—N1B—C1B	−143.30 (16)
O1A—S1A—N1A—C1A	−24.8 (2)	O1B—S1B—N1B—C1B	−11.57 (19)
C8A—S1A—N1A—C1A	88.9 (2)	C8B—S1B—N1B—C1B	102.36 (17)
O2A—S1A—N1A—C4A	2.6 (2)	O2B—S1B—N1B—C4B	−2.67 (19)
O1A—S1A—N1A—C4A	133.44 (19)	O1B—S1B—N1B—C4B	129.07 (17)
C8A—S1A—N1A—C4A	−112.9 (2)	C8B—S1B—N1B—C4B	−117.01 (17)
C4A—N1A—C1A—C2A	−24.3 (3)	C4B—N1B—C1B—C2B	−32.8 (2)
S1A—N1A—C1A—C2A	136.04 (18)	S1B—N1B—C1B—C2B	111.85 (18)
N1A—C1A—C2A—C5A	167.8 (2)	N1B—C1B—C2B—C5B	167.6 (2)
N1A—C1A—C2A—C3A	42.2 (2)	N1B—C1B—C2B—C3B	43.9 (2)
C5A—C2A—C3A—C7A	56.8 (3)	C5B—C2B—C3B—C7B	61.0 (2)
C1A—C2A—C3A—C7A	−173.7 (2)	C1B—C2B—C3B—C7B	−169.79 (19)

C5A—C2A—C3A—C4A	−175.30 (18)	C5B—C2B—C3B—C4B	−169.37 (18)
C1A—C2A—C3A—C4A	−45.8 (2)	C1B—C2B—C3B—C4B	−40.1 (2)
C1A—N1A—C4A—C21A	−127.9 (2)	C1B—N1B—C4B—C21B	−111.4 (2)
S1A—N1A—C4A—C21A	72.2 (3)	S1B—N1B—C4B—C21B	104.7 (2)
C1A—N1A—C4A—C3A	−3.1 (3)	C1B—N1B—C4B—C3B	8.3 (2)
S1A—N1A—C4A—C3A	−162.95 (17)	S1B—N1B—C4B—C3B	−135.65 (17)
C7A—C3A—C4A—N1A	148.0 (2)	C7B—C3B—C4B—N1B	140.7 (2)
C2A—C3A—C4A—N1A	29.3 (2)	C2B—C3B—C4B—N1B	19.8 (2)
C7A—C3A—C4A—C21A	−91.7 (3)	C7B—C3B—C4B—C21B	−99.9 (2)
C2A—C3A—C4A—C21A	149.6 (2)	C2B—C3B—C4B—C21B	139.25 (19)
C6A—O3A—C5A—C2A	31.6 (3)	C6B—O3B—C5B—C16B	−95.6 (2)
C6A—O3A—C5A—C15A	149.7 (2)	C6B—O3B—C5B—C2B	28.0 (3)
C6A—O3A—C5A—C16A	−91.4 (2)	C6B—O3B—C5B—C15B	146.2 (2)
C1A—C2A—C5A—O3A	179.20 (19)	C1B—C2B—C5B—O3B	−178.26 (19)
C3A—C2A—C5A—O3A	−60.2 (2)	C3B—C2B—C5B—O3B	−59.3 (2)
C1A—C2A—C5A—C15A	66.8 (3)	C1B—C2B—C5B—C16B	−59.8 (3)
C3A—C2A—C5A—C15A	−172.64 (19)	C3B—C2B—C5B—C16B	59.1 (3)
C1A—C2A—C5A—C16A	−62.4 (3)	C1B—C2B—C5B—C15B	69.1 (3)
C3A—C2A—C5A—C16A	58.2 (3)	C3B—C2B—C5B—C15B	−171.96 (19)
C5A—O3A—C6A—C7A	−1.6 (4)	C5B—O3B—C6B—C7B	1.2 (4)
C5A—O3A—C6A—N2A	178.30 (19)	C5B—O3B—C6B—N2B	−179.6 (2)
C17A—N2A—C6A—O3A	176.2 (2)	C17B—N2B—C6B—O3B	178.7 (2)
C19A—N2A—C6A—O3A	2.4 (3)	C19B—N2B—C6B—O3B	1.5 (3)
C17A—N2A—C6A—C7A	−4.0 (4)	C17B—N2B—C6B—C7B	−2.0 (4)
C19A—N2A—C6A—C7A	−177.7 (2)	C19B—N2B—C6B—C7B	−179.2 (2)
O3A—C6A—C7A—C18A	176.8 (2)	O3B—C6B—C7B—C18B	178.4 (2)
N2A—C6A—C7A—C18A	−3.0 (4)	N2B—C6B—C7B—C18B	−0.8 (4)
O3A—C6A—C7A—C3A	−2.3 (4)	O3B—C6B—C7B—C3B	0.0 (4)
N2A—C6A—C7A—C3A	177.9 (2)	N2B—C6B—C7B—C3B	−179.2 (2)
C2A—C3A—C7A—C6A	−24.4 (3)	C2B—C3B—C7B—C6B	−29.9 (3)
C4A—C3A—C7A—C6A	−141.0 (2)	C4B—C3B—C7B—C6B	−149.7 (2)
C2A—C3A—C7A—C18A	156.5 (2)	C2B—C3B—C7B—C18B	151.8 (2)
C4A—C3A—C7A—C18A	39.9 (3)	C4B—C3B—C7B—C18B	31.9 (3)
O2A—S1A—C8A—C9A	−8.3 (2)	O2B—S1B—C8B—C9B	−2.6 (2)
O1A—S1A—C8A—C9A	−137.3 (2)	O1B—S1B—C8B—C9B	−132.0 (2)
N1A—S1A—C8A—C9A	107.1 (2)	N1B—S1B—C8B—C9B	112.4 (2)
O2A—S1A—C8A—C13A	171.4 (2)	O2B—S1B—C8B—C13B	179.20 (19)
O1A—S1A—C8A—C13A	42.5 (2)	O1B—S1B—C8B—C13B	49.8 (2)
N1A—S1A—C8A—C13A	−73.1 (2)	N1B—S1B—C8B—C13B	−65.8 (2)
C13A—C8A—C9A—C10A	−0.2 (4)	C13B—C8B—C9B—C10B	0.1 (4)
S1A—C8A—C9A—C10A	179.52 (19)	S1B—C8B—C9B—C10B	−178.11 (19)
C8A—C9A—C10A—C11A	−0.9 (4)	C8B—C9B—C10B—C11B	−0.1 (4)
C9A—C10A—C11A—C12A	1.3 (4)	C9B—C10B—C11B—C12B	−0.2 (4)
C9A—C10A—C11A—C14A	−178.4 (2)	C9B—C10B—C11B—C14B	179.6 (2)
C10A—C11A—C12A—C13A	−0.7 (4)	C10B—C11B—C12B—C13B	0.5 (4)
C14A—C11A—C12A—C13A	179.0 (2)	C14B—C11B—C12B—C13B	−179.3 (2)
C11A—C12A—C13A—C8A	−0.3 (4)	C11B—C12B—C13B—C8B	−0.5 (4)
C9A—C8A—C13A—C12A	0.8 (4)	C9B—C8B—C13B—C12B	0.2 (4)
S1A—C8A—C13A—C12A	−178.93 (19)	S1B—C8B—C13B—C12B	178.37 (18)

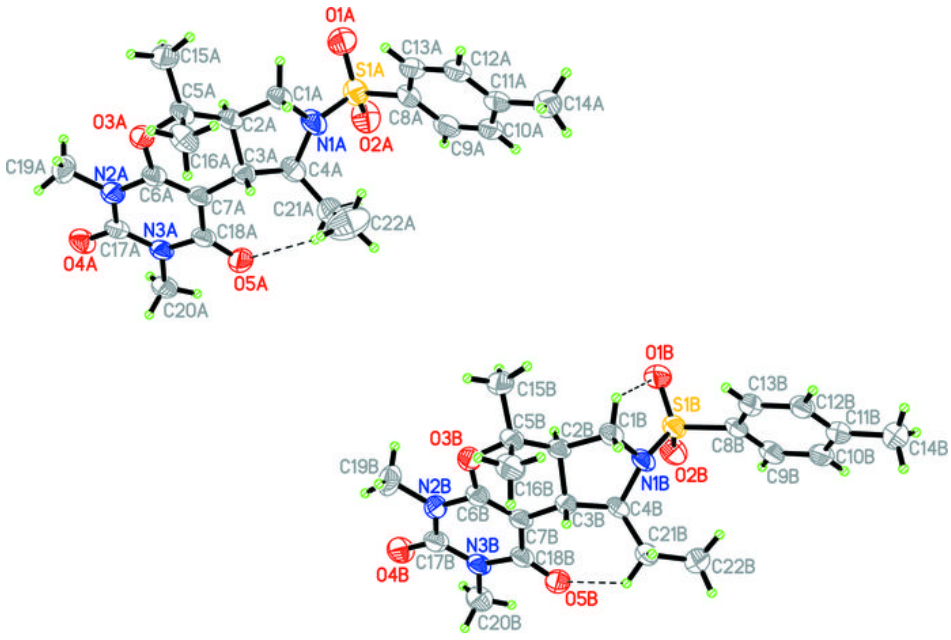
C18A—N3A—C17A—O4A	179.3 (2)	C18B—N3B—C17B—O4B	−178.6 (2)
C20A—N3A—C17A—O4A	0.7 (3)	C20B—N3B—C17B—O4B	1.4 (4)
C18A—N3A—C17A—N2A	−2.6 (3)	C18B—N3B—C17B—N2B	0.7 (4)
C20A—N3A—C17A—N2A	178.8 (2)	C20B—N3B—C17B—N2B	−179.3 (2)
C6A—N2A—C17A—O4A	−175.3 (2)	C6B—N2B—C17B—O4B	−178.7 (2)
C19A—N2A—C17A—O4A	−1.3 (3)	C19B—N2B—C17B—O4B	−1.4 (4)
C6A—N2A—C17A—N3A	6.6 (3)	C6B—N2B—C17B—N3B	2.0 (3)
C19A—N2A—C17A—N3A	−179.4 (2)	C19B—N2B—C17B—N3B	179.3 (2)
C17A—N3A—C18A—O5A	176.6 (2)	C17B—N3B—C18B—O5B	176.9 (2)
C20A—N3A—C18A—O5A	−4.8 (3)	C20B—N3B—C18B—O5B	−3.1 (3)
C17A—N3A—C18A—C7A	−4.0 (3)	C17B—N3B—C18B—C7B	−3.3 (3)
C20A—N3A—C18A—C7A	174.6 (2)	C20B—N3B—C18B—C7B	176.7 (2)
C6A—C7A—C18A—O5A	−173.9 (2)	C6B—C7B—C18B—O5B	−177.0 (2)
C3A—C7A—C18A—O5A	5.2 (4)	C3B—C7B—C18B—O5B	1.3 (4)
C6A—C7A—C18A—N3A	6.7 (3)	C6B—C7B—C18B—N3B	3.2 (3)
C3A—C7A—C18A—N3A	−174.2 (2)	C3B—C7B—C18B—N3B	−178.5 (2)
N1A—C4A—C21A—C22A	56.7 (3)	N1B—C4B—C21B—C22B	−67.7 (3)
C3A—C4A—C21A—C22A	−58.1 (3)	C3B—C4B—C21B—C22B	178.11 (19)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1A—H1B···O4B^{i}	0.97	2.46	3.424 (3)	171
C1B—H1C···O1B	0.97	2.36	2.838 (3)	110
C1B—H1D···O4A^{ii}	0.97	2.40	3.346 (3)	166
C10B—H10B···O5A^{iii}	0.93	2.46	3.374 (3)	168
C15A—H15A···O2A^{iv}	0.96	2.54	3.426 (3)	153
C15B—H15E···O2B^{iii}	0.96	2.55	3.434 (3)	154
C16A—H16C···O4B^{i}	0.96	2.58	3.512 (3)	164
C20B—H20E···O4A^{v}	0.96	2.55	3.387 (3)	145
C21A—H21A···O5A	0.97	2.27	3.040 (3)	136
C21B—H21D···O5B	0.97	2.50	3.152 (3)	125
C21B—H21D···Cg1^{vi}	0.97	2.96	3.591 (3)	123

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

Fig. 1


O1A
C15A
C13A
C12A
S1A
C11A
C14A
C5A
C1A
C8A
C10A
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N1A
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C9A
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Fig. 2

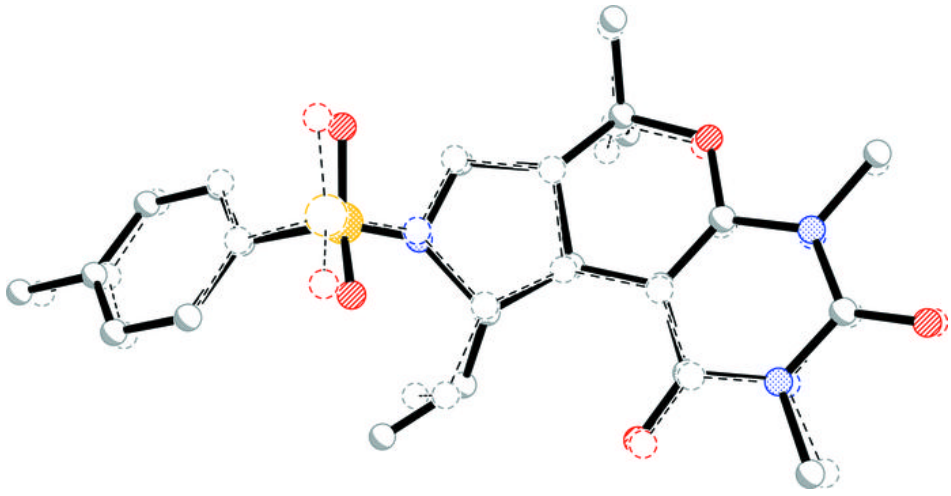
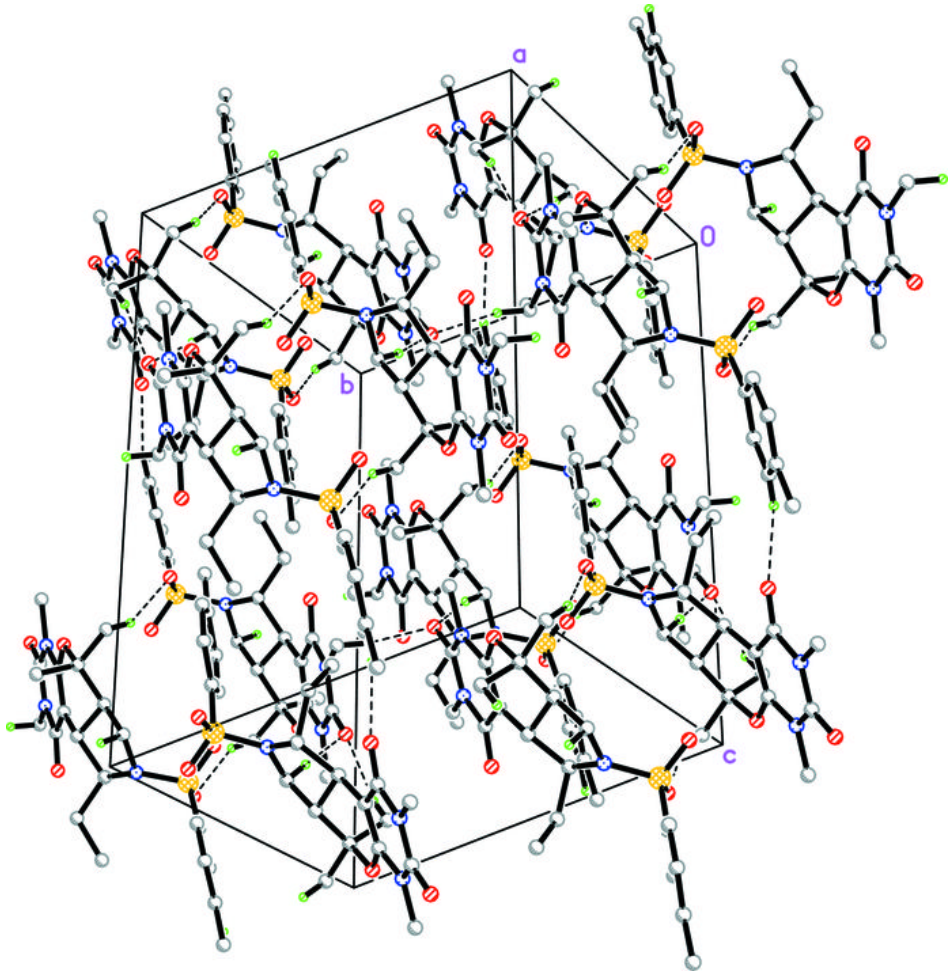


Fig. 3



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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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