Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

K. Chinnakali,[a]‡ D. Sudha,[a]§ M. Jayagopi,[b] R. Raghunathan[b] and Hoong-Kun Fun[c]*

[a]Department of Physics, Anna University, Chennai 600 025, India, [b]Department of Organic Chemistry, University of Madras, Guindy Campus, Chennai 600 025, India, and [c]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia
Correspondence e-mail: hkfun@usm.my

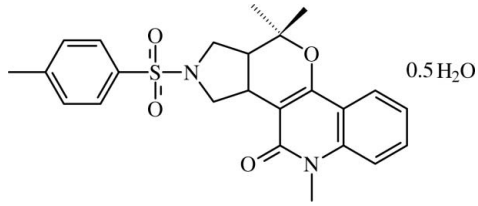
Received 22 October 2007; accepted 25 October 2007

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.053; wR factor = 0.129; data-to-parameter ratio = 22.2.

The asymmetric unit of the title compound, $C_{24}H_{26}N_2O_4S\cdot 0.5H_2O$, contains two independent molecules, *A* and *B*, with similar conformations, and a water molecule. The pyrrolidine ring adopts an envelope conformation in molecule *A* and a twist conformation in molecule *B*. In both molecules, the pyrrolidine and dihydropyran rings are *cis*-fused, and the dihydropyran ring has a half-chair conformation. Each of the independent molecules adopts a folded conformation, with the sulfonyl-bound benzene ring lying over the pyridinone ring. The two independent molecules, *A* and *B*, are linked together *via* C—H···O hydrogen bonds and C—H···π interactions. The *A*–*B* pairs are linked into a chain along the *a* axis by O—H···O and C—H···O hydrogen bonds, as well as C—H···π interactions. The inversion- and screw-related molecules in adjacent chains are cross-linked *via* C—H···O and C—H···N interactions, forming a three-dimensional framework.

Related literature

For biological activities of pyranoquinolinones, see: Butenschön *et al.* (2001); Edwards *et al.* (1999); Hanawa *et al.* (2004); Kamikawa *et al.* (1996); Keenan (1994); Wasserman (1995). For ring puckering parameters, see: Cremer & Pople (1975). For asymmetry parameters, see: Duax *et al.* (1976). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{24}H_{26}N_2O_4S\cdot 0.5H_2O$
M_r = 447.54
Monoclinic, $P2_1/c$
a = 15.1413 (3) Å
b = 14.7008 (3) Å
c = 20.9973 (4) Å
β = 111.336 (1)°
V = 4353.44 (15) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.19 mm^{-1}
T = 100.0 (1) K
0.43 × 0.31 × 0.07 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.914, T_{max} = 0.988
127879 measured reflections
12850 independent reflections
9240 reflections with $I > 2\sigma(I)$
R_{int} = 0.083

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.129
S = 1.07
12850 reflections
580 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}

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

*Cg*1 and *Cg*2 are the centroids of the C8*B*–C13*B* and N2*B*/C22*B*/C17*B*/C6*B*/C7*B*/C23*B* rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
O1*W*—H1O···O2*A*^{i}	0.85 (3)	2.04 (3)	2.879 (3)	167 (3)
O1*W*—H2O···O4*B*	0.85 (3)	2.00 (3)	2.841 (2)	175 (4)
C2*B*—H2*B*···O1*B*^{ii}	0.98	2.59	3.485 (2)	152
C4*A*—H4*A*···N1*A*^{iii}	0.97	2.54	3.356 (2)	142
C4*A*—H4*B*···O4*A*	0.97	2.35	2.927 (2)	117
C4*B*—H4*C*···O4*B*	0.97	2.37	2.976 (2)	120
C14*A*—H14*B*···O1*W*^{iv}	0.96	2.57	3.521 (3)	170
C14*B*—H14*F*···O2*B*^{iv}	0.96	2.52	3.276 (3)	136
C15*A*—H15*A*···O1*B*	0.96	2.55	3.502 (2)	172
C16*B*—H16*D*···O4*A*^{i}	0.96	2.60	3.474 (2)	152
C12*A*—H12*A*···*Cg*1	0.93	2.87	3.684 (2)	147
C24*A*—H24*C*···*Cg*2^{v}	0.96	2.86	3.800 (2)	166

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

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 the Fundamental Research Grant Scheme (FRGS) grant No. 203/PFIZIK/671064.

‡ Additional correspondence author, email: kali@annauniv.edu.
§ Working at Department of Physics, RMK Engineering College, RSM Nagar, Kavaraipettai 601 206, Tamil Nadu, India.

 doi:10.1107/S1600536807053287

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2212).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.

Bruker (2005). *APEX2* (Version 1.27), *SAINT* (Version 7.12a) and *SADABS* (Version 2004/1). Bruker AXS Inc., Madison, Wisconsin, USA.

Butenschön, I., Möller, K. & Hänsel, W. (2001). *J. Med. Chem.* **44**, 1249–1256.

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.

Edwards, J. P., Higuchi, R. I., Winn, D. T., Pooley, C. L., Caferro, T. R., Hamann, L. G., Zhi, L., Marschke, K. B., Goldman, M. E. & Jones, T. K. (1999). *Bioorg. Med. Chem. Lett.* **9**, 1003–1008.

Hanawa, F., Fokialakis, N. & Skaltsounis, A. L. (2004). *Planta Med.* **70**, 531–535.

Kamikawa, T., Hanaoka, Y., Fujie, S., Saito, K., Yamagiwa, Y., Fukuhara, K. & Kubo, I. (1996). *Bioorg. Med. Chem.* **4**, 1317–1320.

Keenan, J. M. (1994). *Am. Fam. Physician*, **50**, 1059–1064.

Sheldrick, G. M. (1998). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.

Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

Wasserman, S. I. (1995). *Allergy Proc.* **16**, 67–71.

supplementary materials

Acta Cryst. (2007). E**63**, o4489-o4490 [**doi:10.1107/S1600536807053287**]

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

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

Comment

Pyranoquinolone alkaloids exhibit photo-activated antimicrobial activity (Hanawa *et al.*, 2004) and SRS-A antagonist action (Kamikawa *et al.*, 1996). 2*H*-Pyrano[3,2-*g*]quinolin-2-one derivatives are found to modulate the transcriptional activity of the human androgen receptor (Edwards *et al.*, 1999). Pyranoquinolinones act as blockers of the voltage-gated potassium channel Kv1.3 (Butenschön *et al.*, 2001). Nedocromil sodium, a pyranoquinolone, was specifically designed as an agent to suppress allergic inflammation (Wasserman 1995). Nedocromil sodium is used as an anti-inflammatory medication for the treatment of mild to moderate asthma (Keenan, 1994). In view of the above biological activities associated with pyranoquinolone derivatives, we have undertaken the crystal structure determination of the title compound.

There are two independent molecules, *A* and *B*, in the asymmetric unit, with 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 0.180 Å. The geometric parameters in *A* and *B* are similar, and show normal values (Allen *et al.*, 1987).

The pyrrolidine ring of molecule A adopts an envelope conformation, with the local mirror plane passing through C2 and the midpoint of the bond N1—C4; the asymmetry parameter (Duax *et al.*, 1976) ΔC_s[C2A] is 5.2 (2)°, and the Cremer & Pople (1975) puckering parameters Q and φ are 0.348 (2) Å and 259.7 (3)°. In molecule B, the pyrrolidine ring adopts a twist conformation, with the local twofold rotation axis passing through atom N1 and the mid-point of the opposite bond C2—C3; the puckering parameters (Cremer & Pople, 1975) are q_2 = 0.369 (2) Å and φ = 91.8 (3)°, and the asymmetry parameter ΔC_2[C2B—C3B] is 1.8 (2)°. The tosyl group is equatorially attached to the pyrrolidine ring in both molecule *A* and molecule *B*. The pyrrolidine ring in both molecules is *cis*-fused to the dihydropyran ring.

In each of the independent molecules, the dihydropyran ring has a half-chair conformation, with a local pseudo-twofold axis running through the midpoints of the C2—C5 and C6—C7 bonds. The puckering parameters Q, θ and φ, and the smallest displacement asymmetry parameters ΔC_2[C2—C5] for the molecules A/B are 0.443 (2)/0.462 (2) Å, 128.7 (2)/53.2 (2)°, 262.5 (3)/88.7 (3)° and 9.0 (2)/3.2 (3)°.

In both molecules, the sulfonyl group has a distorted tetrahedral geometry, with the O1—S1—O2 [119.12 (8)° in A and 120.10 (8)° in B] angle deviating significantly from the ideal tetrahedral value.

The quinolinone ring system is planar, with maximum deviations of 0.060 (1) Å for C23A and 0.042 (1) Å for C6B. The dihedral angle between the quinolinone ring system and the C8—C13 ring is 18.84 (8)° in molecule A and 15.53 (6)° in molecule B. Each of the independent molecules adopts a folded conformation, with the sulfonyl-bound benzene ring lying over the pyridinone ring. The centroid-centroid distance between these rings [3.892 (1) Å in molecule A and 3.709 (1) Å in molecule B] indicate the presence of weak π-π interactions between them.

The two independent molecules, A and B, are linked together *via* the C15A—H15A···O1B hydrogen bond and C12—H12A···π interaction involving the C8B—C13B benzene ring (centroid *Cg*1). The A—B pairs are linked into a

chain along the *a* axis (Fig. 3) by O1W—H1O···O2A^{i}, O1W—H2O···O4B and C16B—H16D···O4A^{i} hydrogen bonds, and C24A—H24C···π interactions involving the N2B/C22B/C17B/C6B/C7B/C23B ring (centroid *Cg*2) of the molecule at (−1 + *x*, *y*, *z*). The inversion- and screw-related molecules in adjacent chains are cross-linked *via* C—H···O and C—H···N type interactions (Table 1) forming a three-dimensional framework (Fig. 4).

Experimental

To a solution of 1-methylquinoline-2,4-dione (1 mmol) in dry toluene (20 ml), 2-[*N*-(3-methylbut-2-enyl)-*N*-tosylamino]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

The water H atoms were located and isotropically refined, with the O—H and H···H distances restrained to 0.84 (1) and 1.37 (2) Å, respectively. The remaining H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93–0.98 Å. The U_{iso} values were set equal to 1.5U_{eq} of the carrier atom for methyl H atoms and 1.2U_{eq} for the remaining H atoms. A rotating group model was used for the methyl groups attached to aromatic rings.

Figures

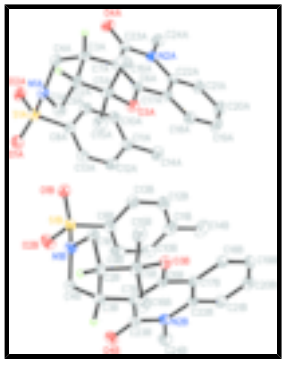


Fig. 1. The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 80% probability level. All H atoms except those at the ring junctions have been omitted for clarity. The solvent water molecule has also been omitted.

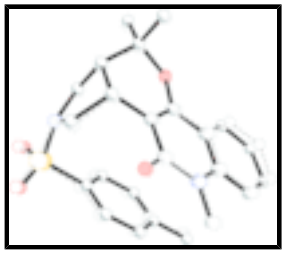


Fig. 2. Fit of molecule A (dashed lines) on molecule B (solid lines). H atoms have been omitted for clarity.

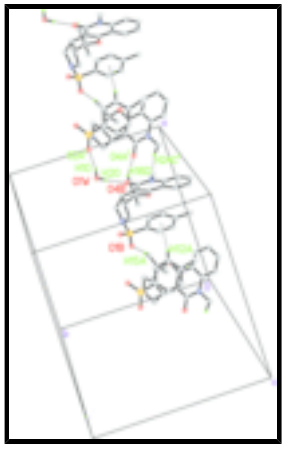


Fig. 3. View of a hydrogen-bonded chain along the *a* axis. Dashed and dotted lines indicate C—H···O and C—H···π interactions, respectively. For the sake of clarity, H atoms not involved in the interactions have been omitted. Symmetry code: (i) 1 + *x*, *y*, *z*.

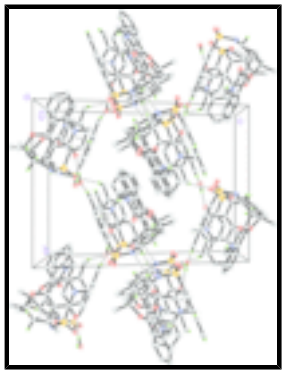


Fig. 4. The crystal packing of the title compound, viewed approximately along the *a* axis. Hydrogen bonds are shown as dashed lines.

cis-4,4,10-Trimethyl-2-tosyl-1,2,3,3a,4,11_b_-hexahydro- 11_H_-pyrrolo[3,4-_c_]pyrano[5,6-_c_]quinolin-11-one hemihydrate

Crystal data

$C_{24}H_{26}N_2O_4S·0.5H_2O$	F_{000} = 1896
M_r = 447.54	D_x = 1.366 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 6683 reflections
a = 15.1413 (3) Å	θ = 2.5–26.8º
b = 14.7008 (3) Å	μ = 0.19 mm^{-1}
c = 20.9973 (4) Å	*T* = 100.0 (1) K
β = 111.336 (1)º	Plate, colourless
V = 4353.44 (15) Å^3	0.43 × 0.31 × 0.07 mm
Z = 8	

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	12850 independent reflections
Radiation source: fine-focus sealed tube	9240 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.083

Detector resolution: 8.33 pixels mm^{-1}

T = 100.0(1) K

ω scans

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

T_{min} = 0.914, T_{max} = 0.988

127879 measured reflections

θ_{max} = 30.2º

θ_{min} = 1.4º

h = −21→21

k = −20→20

l = −29→29

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.053

$wR(F^2)$ = 0.129

S = 1.07

12850 reflections

580 parameters

3 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0482P)^2 + 1.9763P]$ where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max}$ = 0.45 e $Å^{-3}$

$\Delta\rho_{min}$ = −0.48 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}
S1A	0.14006 (3)	0.45280 (3)	0.13902 (2)	0.02455 (10)
O1A	0.21862 (9)	0.51151 (9)	0.14579 (7)	0.0295 (3)
O2A	0.06662 (9)	0.48433 (9)	0.16204 (7)	0.0305 (3)
O3A	0.16268 (8)	0.20335 (8)	−0.02022 (6)	0.0220 (3)
O4A	−0.10267 (9)	0.21723 (9)	0.04918 (7)	0.0303 (3)
N1A	0.08911 (10)	0.42912 (10)	0.05875 (8)	0.0238 (3)
N2A	−0.00010 (10)	0.09761 (10)	0.08325 (8)	0.0223 (3)
C1A	0.14931 (13)	0.39537 (12)	0.02195 (9)	0.0243 (4)

H1A	0.1961	0.3524	0.0497	0.029*
H1B	0.1817	0.4452	0.0093	0.029*
C2A	0.07911 (12)	0.34915 (12)	−0.04138 (9)	0.0236 (4)
H2A	0.0508	0.3954	−0.0766	0.028*
C3A	0.00165 (12)	0.31141 (12)	−0.01682 (9)	0.0238 (4)
H3A	−0.0589	0.3075	−0.0554	0.029*
C4A	−0.00479 (13)	0.38297 (12)	0.03434 (10)	0.0266 (4)
H4A	−0.0552	0.4261	0.0123	0.032*
H4B	−0.0167	0.3545	0.0721	0.032*
C5A	0.12517 (12)	0.27597 (12)	−0.07069 (9)	0.0231 (4)
C6A	0.10534 (12)	0.17262 (11)	0.01219 (8)	0.0195 (3)
C7A	0.02939 (12)	0.21924 (12)	0.01508 (9)	0.0214 (3)
C8A	0.18494 (12)	0.35034 (12)	0.18098 (9)	0.0227 (3)
C9A	0.12682 (13)	0.29190 (13)	0.20070 (9)	0.0257 (4)
H9A	0.0659	0.3098	0.1962	0.031*
C10A	0.16061 (13)	0.20680 (13)	0.22710 (9)	0.0262 (4)
H10A	0.1219	0.1679	0.2403	0.031*
C11A	0.25174 (13)	0.17885 (13)	0.23417 (9)	0.0252 (4)
C12A	0.30890 (13)	0.23906 (13)	0.21522 (9)	0.0256 (4)
H12A	0.3703	0.2217	0.2208	0.031*
C13A	0.27665 (13)	0.32378 (12)	0.18836 (9)	0.0242 (4)
H13A	0.3156	0.3626	0.1754	0.029*
C14A	0.28765 (15)	0.08638 (14)	0.26190 (11)	0.0353 (5)
H14A	0.3045	0.0531	0.2286	0.053*
H14B	0.2390	0.0541	0.2718	0.053*
H14C	0.3424	0.0927	0.3031	0.053*
C15A	0.21092 (13)	0.31180 (13)	−0.08399 (10)	0.0269 (4)
H15A	0.2574	0.3331	−0.0419	0.040*
H15B	0.1919	0.3610	−0.1162	0.040*
H15C	0.2377	0.2639	−0.1023	0.040*
C16A	0.05403 (14)	0.23347 (14)	−0.13521 (9)	0.0308 (4)
H16A	0.0287	0.2797	−0.1693	0.046*
H16B	0.0034	0.2060	−0.1247	0.046*
H16C	0.0852	0.1879	−0.1523	0.046*
C17A	0.13210 (12)	0.08545 (12)	0.04513 (9)	0.0205 (3)
C18A	0.20821 (13)	0.03522 (12)	0.04113 (10)	0.0250 (4)
H18A	0.2428	0.0577	0.0159	0.030*
C19A	0.23268 (14)	−0.04711 (13)	0.07401 (11)	0.0320 (4)
H19A	0.2831	−0.0804	0.0707	0.038*
C20A	0.18144 (15)	−0.08005 (13)	0.11216 (11)	0.0335 (5)
H20A	0.1987	−0.1351	0.1352	0.040*
C21A	0.10536 (13)	−0.03240 (12)	0.11640 (10)	0.0270 (4)
H21A	0.0717	−0.0555	0.1421	0.032*
C22A	0.07879 (12)	0.05025 (12)	0.08230 (9)	0.0210 (3)
C23A	−0.02980 (12)	0.17957 (12)	0.04901 (9)	0.0233 (4)
C24A	−0.05641 (14)	0.05970 (14)	0.12057 (11)	0.0313 (4)
H24A	−0.0168	0.0513	0.1677	0.047*
H24B	−0.0823	0.0021	0.1010	0.047*
H24C	−0.1071	0.1007	0.1175	0.047*

S1B	0.47819 (3)	0.40160 (3)	0.10379 (2)	0.02499 (10)
O1B	0.37993 (9)	0.41034 (9)	0.06117 (7)	0.0292 (3)
O2B	0.51922 (10)	0.46166 (10)	0.16050 (7)	0.0351 (3)
O3B	0.60130 (8)	0.19484 (8)	−0.03158 (6)	0.0219 (3)
O4B	0.80786 (9)	0.32524 (9)	0.17597 (7)	0.0306 (3)
N1B	0.53778 (10)	0.41522 (10)	0.05437 (8)	0.0228 (3)
N2B	0.77630 (10)	0.17361 (10)	0.17130 (7)	0.0223 (3)
C1B	0.50881 (12)	0.36308 (12)	−0.01021 (9)	0.0227 (3)
H1C	0.4575	0.3934	−0.0460	0.027*
H1D	0.4886	0.3022	−0.0040	0.027*
C2B	0.59851 (12)	0.36028 (12)	−0.02754 (9)	0.0223 (3)
H2B	0.6010	0.4155	−0.0530	0.027*
C3B	0.68005 (12)	0.36293 (12)	0.04217 (9)	0.0224 (3)
H3B	0.7376	0.3875	0.0376	0.027*
C4B	0.64203 (12)	0.42851 (12)	0.08300 (10)	0.0240 (4)
H4C	0.6676	0.4138	0.1313	0.029*
H4D	0.6584	0.4909	0.0770	0.029*
C5B	0.60273 (13)	0.27799 (12)	−0.07003 (9)	0.0232 (4)
C6B	0.65685 (11)	0.19375 (11)	0.03574 (9)	0.0192 (3)
C7B	0.69778 (12)	0.26877 (12)	0.07220 (9)	0.0207 (3)
C8B	0.49470 (12)	0.28906 (12)	0.13458 (9)	0.0239 (4)
C9B	0.57094 (13)	0.26678 (15)	0.19336 (10)	0.0304 (4)
H9B	0.6132	0.3116	0.2175	0.036*
C10B	0.58383 (14)	0.17739 (15)	0.21592 (10)	0.0331 (5)
H10B	0.6351	0.1631	0.2554	0.040*
C11B	0.52219 (14)	0.10874 (14)	0.18116 (10)	0.0300 (4)
C12B	0.44614 (14)	0.13244 (13)	0.12210 (10)	0.0279 (4)
H12B	0.4042	0.0874	0.0979	0.033*
C13B	0.43149 (13)	0.22120 (13)	0.09861 (9)	0.0253 (4)
H13B	0.3801	0.2356	0.0593	0.030*
C14B	0.53447 (17)	0.01261 (15)	0.20603 (12)	0.0412 (5)
H14D	0.5956	0.0058	0.2416	0.062*
H14E	0.5298	−0.0275	0.1689	0.062*
H14F	0.4859	−0.0022	0.2236	0.062*
C15B	0.51537 (14)	0.27001 (13)	−0.13491 (9)	0.0285 (4)
H15D	0.4596	0.2692	−0.1234	0.043*
H15E	0.5187	0.2147	−0.1583	0.043*
H15F	0.5126	0.3211	−0.1641	0.043*
C16B	0.69318 (13)	0.27949 (13)	−0.08609 (10)	0.0275 (4)
H16D	0.7472	0.2846	−0.0443	0.041*
H16E	0.6916	0.3306	−0.1150	0.041*
H16F	0.6977	0.2243	−0.1091	0.041*
C17B	0.66912 (11)	0.10497 (11)	0.06711 (9)	0.0193 (3)
C18B	0.62176 (12)	0.02760 (12)	0.03222 (9)	0.0222 (3)
H18B	0.5806	0.0328	−0.0130	0.027*
C19B	0.63532 (13)	−0.05610 (12)	0.06392 (9)	0.0246 (4)
H19B	0.6027	−0.1069	0.0406	0.029*
C20B	0.69838 (13)	−0.06385 (12)	0.13126 (9)	0.0257 (4)
H20B	0.7089	−0.1205	0.1524	0.031*

C21B	0.74517 (13)	0.01096 (12)	0.16682 (9)	0.0241 (4)
H21B	0.7871	0.0045	0.2117	0.029*
C22B	0.73014 (11)	0.09692 (12)	0.13589 (9)	0.0200 (3)
C23B	0.76385 (12)	0.25941 (12)	0.14211 (9)	0.0233 (4)
C24B	0.84027 (14)	0.16475 (14)	0.24276 (10)	0.0309 (4)
H24D	0.8640	0.2237	0.2606	0.046*
H24E	0.8924	0.1258	0.2453	0.046*
H24F	0.8064	0.1390	0.2692	0.046*
O1W	0.90357 (15)	0.49532 (13)	0.20138 (13)	0.0656 (6)
H1O	0.9533 (15)	0.484 (2)	0.1929 (18)	0.101 (13)*
H2O	0.873 (2)	0.4457 (15)	0.195 (2)	0.127 (16)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1A	0.0280 (2)	0.0203 (2)	0.0278 (2)	0.00348 (17)	0.01312 (19)	0.00070 (18)
O1A	0.0332 (7)	0.0231 (7)	0.0351 (7)	−0.0024 (5)	0.0157 (6)	−0.0020 (6)
O2A	0.0323 (7)	0.0264 (7)	0.0370 (8)	0.0061 (6)	0.0175 (6)	−0.0025 (6)
O3A	0.0217 (6)	0.0228 (6)	0.0237 (6)	0.0022 (5)	0.0109 (5)	0.0037 (5)
O4A	0.0203 (6)	0.0318 (7)	0.0415 (8)	0.0042 (5)	0.0145 (6)	0.0022 (6)
N1A	0.0245 (7)	0.0223 (7)	0.0256 (8)	0.0036 (6)	0.0104 (6)	0.0018 (6)
N2A	0.0193 (7)	0.0230 (7)	0.0269 (8)	0.0008 (6)	0.0111 (6)	0.0012 (6)
C1A	0.0258 (9)	0.0227 (9)	0.0265 (9)	0.0017 (7)	0.0120 (7)	0.0017 (7)
C2A	0.0229 (8)	0.0224 (9)	0.0247 (9)	0.0038 (7)	0.0077 (7)	0.0049 (7)
C3A	0.0185 (8)	0.0279 (9)	0.0230 (8)	0.0034 (7)	0.0053 (7)	0.0039 (7)
C4A	0.0238 (9)	0.0227 (9)	0.0346 (10)	0.0056 (7)	0.0121 (8)	0.0033 (8)
C5A	0.0232 (8)	0.0248 (9)	0.0198 (8)	0.0020 (7)	0.0061 (7)	0.0043 (7)
C6A	0.0189 (8)	0.0205 (8)	0.0188 (8)	−0.0014 (6)	0.0064 (6)	−0.0019 (6)
C7A	0.0179 (8)	0.0228 (9)	0.0223 (8)	0.0007 (6)	0.0058 (7)	−0.0007 (7)
C8A	0.0240 (8)	0.0239 (9)	0.0203 (8)	0.0018 (7)	0.0082 (7)	−0.0007 (7)
C9A	0.0237 (9)	0.0301 (10)	0.0232 (9)	0.0025 (7)	0.0083 (7)	0.0030 (7)
C10A	0.0257 (9)	0.0288 (10)	0.0242 (9)	−0.0033 (7)	0.0089 (7)	0.0031 (7)
C11A	0.0276 (9)	0.0253 (9)	0.0198 (8)	0.0019 (7)	0.0050 (7)	0.0011 (7)
C12A	0.0238 (9)	0.0306 (10)	0.0220 (9)	0.0036 (7)	0.0080 (7)	0.0005 (7)
C13A	0.0245 (9)	0.0261 (9)	0.0225 (8)	−0.0005 (7)	0.0089 (7)	0.0007 (7)
C14A	0.0346 (11)	0.0291 (11)	0.0391 (11)	0.0046 (8)	0.0100 (9)	0.0077 (9)
C15A	0.0285 (9)	0.0279 (10)	0.0261 (9)	−0.0018 (7)	0.0120 (8)	0.0010 (8)
C16A	0.0284 (10)	0.0391 (11)	0.0216 (9)	−0.0047 (8)	0.0051 (8)	−0.0005 (8)
C17A	0.0208 (8)	0.0196 (8)	0.0214 (8)	−0.0013 (6)	0.0079 (7)	−0.0024 (7)
C18A	0.0243 (9)	0.0232 (9)	0.0318 (10)	0.0003 (7)	0.0153 (8)	−0.0008 (7)
C19A	0.0333 (10)	0.0237 (9)	0.0469 (12)	0.0082 (8)	0.0242 (9)	0.0033 (9)
C20A	0.0392 (11)	0.0221 (9)	0.0474 (12)	0.0066 (8)	0.0256 (10)	0.0080 (9)
C21A	0.0298 (9)	0.0215 (9)	0.0354 (10)	0.0003 (7)	0.0187 (8)	0.0019 (8)
C22A	0.0186 (8)	0.0204 (8)	0.0247 (8)	−0.0010 (6)	0.0086 (7)	−0.0040 (7)
C23A	0.0173 (8)	0.0249 (9)	0.0260 (9)	−0.0004 (7)	0.0058 (7)	−0.0021 (7)
C24A	0.0274 (10)	0.0331 (11)	0.0415 (11)	0.0010 (8)	0.0222 (9)	0.0036 (9)
S1B	0.0252 (2)	0.0227 (2)	0.0307 (2)	−0.00265 (17)	0.01445 (19)	−0.00700 (18)
O1B	0.0238 (6)	0.0238 (7)	0.0427 (8)	0.0015 (5)	0.0153 (6)	−0.0019 (6)

O2B	0.0387 (8)	0.0342 (8)	0.0382 (8)	−0.0102 (6)	0.0209 (7)	−0.0169 (6)
O3B	0.0258 (6)	0.0191 (6)	0.0200 (6)	0.0014 (5)	0.0073 (5)	−0.0002 (5)
O4B	0.0277 (7)	0.0250 (7)	0.0326 (7)	−0.0059 (5)	0.0033 (6)	−0.0041 (6)
N1B	0.0208 (7)	0.0219 (7)	0.0271 (8)	−0.0018 (6)	0.0104 (6)	−0.0042 (6)
N2B	0.0194 (7)	0.0233 (8)	0.0217 (7)	−0.0001 (6)	0.0045 (6)	−0.0003 (6)
C1B	0.0207 (8)	0.0211 (9)	0.0262 (9)	0.0022 (7)	0.0083 (7)	−0.0030 (7)
C2B	0.0227 (8)	0.0179 (8)	0.0278 (9)	0.0031 (7)	0.0110 (7)	0.0019 (7)
C3B	0.0196 (8)	0.0189 (8)	0.0297 (9)	−0.0006 (6)	0.0102 (7)	0.0007 (7)
C4B	0.0207 (8)	0.0200 (8)	0.0311 (9)	−0.0018 (7)	0.0091 (7)	−0.0033 (7)
C5B	0.0268 (9)	0.0192 (8)	0.0253 (9)	0.0043 (7)	0.0116 (7)	0.0040 (7)
C6B	0.0162 (7)	0.0210 (8)	0.0217 (8)	0.0026 (6)	0.0083 (6)	0.0009 (7)
C7B	0.0182 (8)	0.0201 (8)	0.0255 (9)	−0.0001 (6)	0.0101 (7)	−0.0008 (7)
C8B	0.0236 (9)	0.0268 (9)	0.0244 (9)	−0.0014 (7)	0.0124 (7)	−0.0038 (7)
C9B	0.0248 (9)	0.0423 (12)	0.0252 (9)	−0.0049 (8)	0.0104 (8)	−0.0035 (8)
C10B	0.0264 (10)	0.0529 (13)	0.0213 (9)	0.0048 (9)	0.0103 (8)	0.0052 (9)
C11B	0.0336 (10)	0.0345 (11)	0.0296 (10)	0.0071 (8)	0.0208 (8)	0.0046 (8)
C12B	0.0328 (10)	0.0246 (9)	0.0301 (10)	0.0000 (8)	0.0158 (8)	−0.0008 (8)
C13B	0.0243 (9)	0.0267 (9)	0.0247 (9)	−0.0001 (7)	0.0085 (7)	−0.0020 (7)
C14B	0.0490 (13)	0.0421 (13)	0.0419 (12)	0.0151 (10)	0.0278 (11)	0.0143 (10)
C15B	0.0332 (10)	0.0260 (10)	0.0247 (9)	0.0068 (8)	0.0088 (8)	0.0011 (8)
C16B	0.0313 (10)	0.0269 (9)	0.0285 (9)	0.0077 (8)	0.0158 (8)	0.0048 (8)
C17B	0.0179 (8)	0.0191 (8)	0.0229 (8)	0.0006 (6)	0.0099 (7)	−0.0002 (7)
C18B	0.0221 (8)	0.0224 (9)	0.0236 (8)	0.0003 (7)	0.0101 (7)	−0.0025 (7)
C19B	0.0284 (9)	0.0189 (8)	0.0297 (9)	−0.0038 (7)	0.0146 (8)	−0.0035 (7)
C20B	0.0317 (10)	0.0206 (9)	0.0282 (9)	0.0031 (7)	0.0149 (8)	0.0034 (7)
C21B	0.0252 (9)	0.0253 (9)	0.0213 (8)	0.0024 (7)	0.0080 (7)	0.0022 (7)
C22B	0.0171 (8)	0.0218 (8)	0.0226 (8)	0.0001 (6)	0.0089 (6)	−0.0013 (7)
C23B	0.0198 (8)	0.0227 (9)	0.0273 (9)	−0.0008 (7)	0.0086 (7)	−0.0019 (7)
C24B	0.0289 (10)	0.0319 (11)	0.0246 (9)	0.0006 (8)	0.0009 (8)	−0.0005 (8)
O1W	0.0626 (12)	0.0398 (10)	0.1209 (18)	−0.0162 (9)	0.0649 (13)	−0.0253 (11)

Geometric parameters (Å, °)

S1A—O1A	1.4342 (14)	S1B—O1B	1.4360 (14)
S1A—O2A	1.4407 (13)	S1B—N1B	1.6163 (15)
S1A—N1A	1.6160 (16)	S1B—C8B	1.7607 (19)
S1A—C8A	1.7525 (18)	O3B—C6B	1.357 (2)
O3A—C6A	1.3605 (19)	O3B—C5B	1.469 (2)
O3A—C5A	1.465 (2)	O4B—C23B	1.241 (2)
O4A—C23A	1.236 (2)	N1B—C1B	1.478 (2)
N1A—C1A	1.479 (2)	N1B—C4B	1.483 (2)
N1A—C4A	1.488 (2)	N2B—C23B	1.385 (2)
N2A—C22A	1.389 (2)	N2B—C22B	1.391 (2)
N2A—C23A	1.391 (2)	N2B—C24B	1.466 (2)
N2A—C24A	1.462 (2)	C1B—C2B	1.529 (2)
C1A—C2A	1.527 (3)	C1B—H1C	0.97
C1A—H1A	0.97	C1B—H1D	0.97
C1A—H1B	0.97	C2B—C5B	1.518 (2)
C2A—C5A	1.528 (2)	C2B—C3B	1.534 (2)

C2A—C3A	1.546 (2)	C2B—H2B	0.98
C2A—H2A	0.98	C3B—C7B	1.504 (2)
C3A—C7A	1.502 (2)	C3B—C4B	1.535 (2)
C3A—C4A	1.532 (3)	C3B—H3B	0.98
C3A—H3A	0.98	C4B—H4C	0.97
C4A—H4A	0.97	C4B—H4D	0.97
C4A—H4B	0.97	C5B—C15B	1.519 (3)
C5A—C15A	1.518 (2)	C5B—C16B	1.525 (2)
C5A—C16A	1.525 (3)	C6B—C7B	1.357 (2)
C6A—C7A	1.359 (2)	C6B—C17B	1.443 (2)
C6A—C17A	1.442 (2)	C7B—C23B	1.451 (2)
C7A—C23A	1.454 (2)	C8B—C9B	1.388 (3)
C8A—C13A	1.396 (2)	C8B—C13B	1.398 (3)
C8A—C9A	1.396 (2)	C9B—C10B	1.386 (3)
C9A—C10A	1.389 (3)	C9B—H9B	0.93
C9A—H9A	0.93	C10B—C11B	1.388 (3)
C10A—C11A	1.395 (3)	C10B—H10B	0.93
C10A—H10A	0.93	C11B—C12B	1.395 (3)
C11A—C12A	1.393 (3)	C11B—C14B	1.494 (3)
C11A—C14A	1.501 (3)	C12B—C13B	1.384 (3)
C12A—C13A	1.381 (3)	C12B—H12B	0.93
C12A—H12A	0.93	C13B—H13B	0.93
C13A—H13A	0.93	C14B—H14D	0.96
C14A—H14A	0.96	C14B—H14E	0.96
C14A—H14B	0.96	C14B—H14F	0.96
C14A—H14C	0.96	C15B—H15D	0.96
C15A—H15A	0.96	C15B—H15E	0.96
C15A—H15B	0.96	C15B—H15F	0.96
C15A—H15C	0.96	C16B—H16D	0.96
C16A—H16A	0.96	C16B—H16E	0.96
C16A—H16B	0.96	C16B—H16F	0.96
C16A—H16C	0.96	C17B—C18B	1.401 (2)
C17A—C18A	1.397 (2)	C17B—C22B	1.408 (2)
C17A—C22A	1.410 (2)	C18B—C19B	1.378 (2)
C18A—C19A	1.376 (3)	C18B—H18B	0.93
C18A—H18A	0.93	C19B—C20B	1.393 (3)
C19A—C20A	1.389 (3)	C19B—H19B	0.93
C19A—H19A	0.93	C20B—C21B	1.373 (3)
C20A—C21A	1.378 (3)	C20B—H20B	0.93
C20A—H20A	0.93	C21B—C22B	1.401 (2)
C21A—C22A	1.393 (3)	C21B—H21B	0.93
C21A—H21A	0.93	C24B—H24D	0.96
C24A—H24A	0.96	C24B—H24E	0.96
C24A—H24B	0.96	C24B—H24F	0.96
C24A—H24C	0.96	O1W—H1O	0.851 (10)
S1B—O2B	1.4300 (14)	O1W—H2O	0.850 (10)
O1A—S1A—O2A	119.12 (8)	O2B—S1B—N1B	106.46 (8)
O1A—S1A—N1A	107.27 (8)	O1B—S1B—N1B	106.41 (8)
O2A—S1A—N1A	106.58 (8)	O2B—S1B—C8B	108.29 (9)

O1A—S1A—C8A	108.15 (8)	O1B—S1B—C8B	106.82 (8)
O2A—S1A—C8A	108.26 (8)	N1B—S1B—C8B	108.31 (8)
N1A—S1A—C8A	106.85 (8)	C6B—O3B—C5B	117.06 (13)
C6A—O3A—C5A	116.98 (13)	C1B—N1B—C4B	110.90 (13)
C1A—N1A—C4A	111.13 (14)	C1B—N1B—S1B	118.43 (11)
C1A—N1A—S1A	117.79 (12)	C4B—N1B—S1B	121.09 (12)
C4A—N1A—S1A	119.42 (12)	C23B—N2B—C22B	122.74 (14)
C22A—N2A—C23A	123.01 (14)	C23B—N2B—C24B	117.81 (15)
C22A—N2A—C24A	119.26 (15)	C22B—N2B—C24B	119.44 (15)
C23A—N2A—C24A	117.72 (14)	N1B—C1B—C2B	103.85 (13)
N1A—C1A—C2A	103.78 (14)	N1B—C1B—H1C	111.0
N1A—C1A—H1A	111.0	C2B—C1B—H1C	111.0
C2A—C1A—H1A	111.0	N1B—C1B—H1D	111.0
N1A—C1A—H1B	111.0	C2B—C1B—H1D	111.0
C2A—C1A—H1B	111.0	H1C—C1B—H1D	109.0
H1A—C1A—H1B	109.0	C5B—C2B—C1B	113.10 (14)
C1A—C2A—C5A	112.89 (14)	C5B—C2B—C3B	112.93 (14)
C1A—C2A—C3A	103.98 (14)	C1B—C2B—C3B	104.38 (14)
C5A—C2A—C3A	113.24 (15)	C5B—C2B—H2B	108.7
C1A—C2A—H2A	108.8	C1B—C2B—H2B	108.7
C5A—C2A—H2A	108.8	C3B—C2B—H2B	108.7
C3A—C2A—H2A	108.8	C7B—C3B—C2B	109.60 (14)
C7A—C3A—C4A	112.68 (15)	C7B—C3B—C4B	112.95 (14)
C7A—C3A—C2A	110.46 (14)	C2B—C3B—C4B	102.34 (13)
C4A—C3A—C2A	103.70 (15)	C7B—C3B—H3B	110.6
C7A—C3A—H3A	109.9	C2B—C3B—H3B	110.6
C4A—C3A—H3A	109.9	C4B—C3B—H3B	110.6
C2A—C3A—H3A	109.9	N1B—C4B—C3B	104.54 (14)
N1A—C4A—C3A	104.96 (14)	N1B—C4B—H4C	110.8
N1A—C4A—H4A	110.8	C3B—C4B—H4C	110.8
C3A—C4A—H4A	110.8	N1B—C4B—H4D	110.8
N1A—C4A—H4B	110.8	C3B—C4B—H4D	110.8
C3A—C4A—H4B	110.8	H4C—C4B—H4D	108.9
H4A—C4A—H4B	108.8	O3B—C5B—C2B	109.13 (13)
O3A—C5A—C15A	104.68 (13)	O3B—C5B—C15B	104.27 (14)
O3A—C5A—C16A	107.86 (14)	C2B—C5B—C15B	112.29 (14)
C15A—C5A—C16A	110.72 (15)	O3B—C5B—C16B	109.12 (14)
O3A—C5A—C2A	109.58 (13)	C2B—C5B—C16B	110.58 (15)
C15A—C5A—C2A	112.09 (15)	C15B—C5B—C16B	111.21 (15)
C16A—C5A—C2A	111.59 (15)	O3B—C6B—C7B	124.12 (15)
C7A—C6A—O3A	124.01 (16)	O3B—C6B—C17B	114.47 (14)
C7A—C6A—C17A	121.42 (15)	C7B—C6B—C17B	121.40 (15)
O3A—C6A—C17A	114.56 (14)	C6B—C7B—C23B	119.92 (16)
C6A—C7A—C23A	120.12 (16)	C6B—C7B—C3B	122.43 (16)
C6A—C7A—C3A	122.61 (15)	C23B—C7B—C3B	117.61 (15)
C23A—C7A—C3A	117.26 (15)	C9B—C8B—C13B	119.75 (18)
C13A—C8A—C9A	120.26 (17)	C9B—C8B—S1B	120.61 (15)
C13A—C8A—S1A	118.97 (14)	C13B—C8B—S1B	119.62 (14)
C9A—C8A—S1A	120.46 (13)	C10B—C9B—C8B	119.71 (18)

C10A—C9A—C8A	119.50 (17)	C10B—C9B—H9B	120.1
C10A—C9A—H9A	120.3	C8B—C9B—H9B	120.1
C8A—C9A—H9A	120.3	C9B—C10B—C11B	121.69 (18)
C9A—C10A—C11A	120.96 (17)	C9B—C10B—H10B	119.2
C9A—C10A—H10A	119.5	C11B—C10B—H10B	119.2
C11A—C10A—H10A	119.5	C10B—C11B—C12B	117.74 (18)
C12A—C11A—C10A	118.41 (17)	C10B—C11B—C14B	121.96 (19)
C12A—C11A—C14A	120.74 (17)	C12B—C11B—C14B	120.29 (19)
C10A—C11A—C14A	120.85 (17)	C13B—C12B—C11B	121.71 (18)
C13A—C12A—C11A	121.70 (17)	C13B—C12B—H12B	119.1
C13A—C12A—H12A	119.2	C11B—C12B—H12B	119.1
C11A—C12A—H12A	119.2	C12B—C13B—C8B	119.39 (17)
C12A—C13A—C8A	119.16 (17)	C12B—C13B—H13B	120.3
C12A—C13A—H13A	120.4	C8B—C13B—H13B	120.3
C8A—C13A—H13A	120.4	C11B—C14B—H14D	109.5
C11A—C14A—H14A	109.5	C11B—C14B—H14E	109.5
C11A—C14A—H14B	109.5	H14D—C14B—H14E	109.5
H14A—C14A—H14B	109.5	C11B—C14B—H14F	109.5
C11A—C14A—H14C	109.5	H14D—C14B—H14F	109.5
H14A—C14A—H14C	109.5	H14E—C14B—H14F	109.5
H14B—C14A—H14C	109.5	C5B—C15B—H15D	109.5
C5A—C15A—H15A	109.5	C5B—C15B—H15E	109.5
C5A—C15A—H15B	109.5	H15D—C15B—H15E	109.5
H15A—C15A—H15B	109.5	C5B—C15B—H15F	109.5
C5A—C15A—H15C	109.5	H15D—C15B—H15F	109.5
H15A—C15A—H15C	109.5	H15E—C15B—H15F	109.5
H15B—C15A—H15C	109.5	C5B—C16B—H16D	109.5
C5A—C16A—H16A	109.5	C5B—C16B—H16E	109.5
C5A—C16A—H16B	109.5	H16D—C16B—H16E	109.5
H16A—C16A—H16B	109.5	C5B—C16B—H16F	109.5
C5A—C16A—H16C	109.5	H16D—C16B—H16F	109.5
H16A—C16A—H16C	109.5	H16E—C16B—H16F	109.5
H16B—C16A—H16C	109.5	C18B—C17B—C22B	119.22 (16)
C18A—C17A—C22A	119.37 (16)	C18B—C17B—C6B	122.63 (16)
C18A—C17A—C6A	122.34 (15)	C22B—C17B—C6B	118.14 (15)
C22A—C17A—C6A	118.29 (15)	C19B—C18B—C17B	120.95 (17)
C19A—C18A—C17A	120.82 (16)	C19B—C18B—H18B	119.5
C19A—C18A—H18A	119.6	C17B—C18B—H18B	119.5
C17A—C18A—H18A	119.6	C18B—C19B—C20B	119.32 (17)
C18A—C19A—C20A	119.40 (17)	C18B—C19B—H19B	120.3
C18A—C19A—H19A	120.3	C20B—C19B—H19B	120.3
C20A—C19A—H19A	120.3	C21B—C20B—C19B	120.93 (17)
C21A—C20A—C19A	121.01 (18)	C21B—C20B—H20B	119.5
C21A—C20A—H20A	119.5	C19B—C20B—H20B	119.5
C19A—C20A—H20A	119.5	C20B—C21B—C22B	120.39 (17)
C20A—C21A—C22A	120.12 (17)	C20B—C21B—H21B	119.8
C20A—C21A—H21A	119.9	C22B—C21B—H21B	119.8
C22A—C21A—H21A	119.9	N2B—C22B—C21B	121.21 (15)
N2A—C22A—C21A	121.26 (15)	N2B—C22B—C17B	119.66 (15)

N2A—C22A—C17A	119.52 (16)	C21B—C22B—C17B	119.11 (16)
C21A—C22A—C17A	119.22 (15)	O4B—C23B—N2B	119.88 (16)
O4A—C23A—N2A	120.51 (16)	O4B—C23B—C7B	122.29 (17)
O4A—C23A—C7A	122.12 (17)	N2B—C23B—C7B	117.82 (15)
N2A—C23A—C7A	117.35 (15)	N2B—C24B—H24D	109.5
N2A—C24A—H24A	109.5	N2B—C24B—H24E	109.5
N2A—C24A—H24B	109.5	H24D—C24B—H24E	109.5
H24A—C24A—H24B	109.5	N2B—C24B—H24F	109.5
N2A—C24A—H24C	109.5	H24D—C24B—H24F	109.5
H24A—C24A—H24C	109.5	H24E—C24B—H24F	109.5
H24B—C24A—H24C	109.5	H1O—O1W—H2O	106 (2)
O2B—S1B—O1B	120.10 (8)		
O1A—S1A—N1A—C1A	51.02 (15)	O2B—S1B—N1B—C1B	−178.14 (13)
O2A—S1A—N1A—C1A	179.65 (13)	O1B—S1B—N1B—C1B	−48.94 (15)
C8A—S1A—N1A—C1A	−64.77 (14)	C8B—S1B—N1B—C1B	65.60 (15)
O1A—S1A—N1A—C4A	−169.09 (12)	O2B—S1B—N1B—C4B	38.71 (15)
O2A—S1A—N1A—C4A	−40.46 (15)	O1B—S1B—N1B—C4B	167.91 (13)
C8A—S1A—N1A—C4A	75.13 (14)	C8B—S1B—N1B—C4B	−77.55 (15)
C4A—N1A—C1A—C2A	17.52 (18)	C4B—N1B—C1B—C2B	−10.54 (18)
S1A—N1A—C1A—C2A	160.54 (12)	S1B—N1B—C1B—C2B	−157.19 (12)
N1A—C1A—C2A—C5A	−155.25 (14)	N1B—C1B—C2B—C5B	153.07 (14)
N1A—C1A—C2A—C3A	−32.13 (17)	N1B—C1B—C2B—C3B	29.93 (17)
C1A—C2A—C3A—C7A	−85.93 (17)	C5B—C2B—C3B—C7B	−40.79 (19)
C5A—C2A—C3A—C7A	37.0 (2)	C1B—C2B—C3B—C7B	82.46 (16)
C1A—C2A—C3A—C4A	35.04 (17)	C5B—C2B—C3B—C4B	−160.90 (14)
C5A—C2A—C3A—C4A	157.93 (14)	C1B—C2B—C3B—C4B	−37.65 (17)
C1A—N1A—C4A—C3A	4.42 (19)	C1B—N1B—C4B—C3B	−12.96 (19)
S1A—N1A—C4A—C3A	−137.92 (13)	S1B—N1B—C4B—C3B	132.67 (13)
C7A—C3A—C4A—N1A	95.22 (17)	C7B—C3B—C4B—N1B	−86.91 (17)
C2A—C3A—C4A—N1A	−24.25 (17)	C2B—C3B—C4B—N1B	30.83 (17)
C6A—O3A—C5A—C15A	165.96 (14)	C6B—O3B—C5B—C2B	−43.60 (18)
C6A—O3A—C5A—C16A	−76.09 (18)	C6B—O3B—C5B—C15B	−163.77 (13)
C6A—O3A—C5A—C2A	45.58 (19)	C6B—O3B—C5B—C16B	77.33 (17)
C1A—C2A—C5A—O3A	62.57 (18)	C1B—C2B—C5B—O3B	−60.43 (18)
C3A—C2A—C5A—O3A	−55.24 (18)	C3B—C2B—C5B—O3B	57.84 (18)
C1A—C2A—C5A—C15A	−53.19 (19)	C1B—C2B—C5B—C15B	54.7 (2)
C3A—C2A—C5A—C15A	−171.01 (14)	C3B—C2B—C5B—C15B	172.93 (15)
C1A—C2A—C5A—C16A	−178.03 (15)	C1B—C2B—C5B—C16B	179.52 (14)
C3A—C2A—C5A—C16A	64.15 (19)	C3B—C2B—C5B—C16B	−62.20 (19)
C5A—O3A—C6A—C7A	−18.5 (2)	C5B—O3B—C6B—C7B	13.7 (2)
C5A—O3A—C6A—C17A	162.42 (14)	C5B—O3B—C6B—C17B	−166.89 (13)
O3A—C6A—C7A—C23A	177.94 (15)	O3B—C6B—C7B—C23B	−173.65 (15)
C17A—C6A—C7A—C23A	−3.1 (3)	C17B—C6B—C7B—C23B	7.0 (2)
O3A—C6A—C7A—C3A	−1.0 (3)	O3B—C6B—C7B—C3B	4.2 (2)
C17A—C6A—C7A—C3A	178.04 (16)	C17B—C6B—C7B—C3B	−175.17 (15)
C4A—C3A—C7A—C6A	−124.54 (18)	C2B—C3B—C7B—C6B	10.1 (2)
C2A—C3A—C7A—C6A	−9.1 (2)	C4B—C3B—C7B—C6B	123.54 (17)
C4A—C3A—C7A—C23A	56.5 (2)	C2B—C3B—C7B—C23B	−171.96 (14)
C2A—C3A—C7A—C23A	171.99 (15)	C4B—C3B—C7B—C23B	−58.6 (2)

O1A—S1A—C8A—C13A	−25.67 (17)	O2B—S1B—C8B—C9B	−27.72 (17)
O2A—S1A—C8A—C13A	−156.01 (14)	O1B—S1B—C8B—C9B	−158.39 (14)
N1A—S1A—C8A—C13A	89.53 (15)	N1B—S1B—C8B—C9B	87.35 (16)
O1A—S1A—C8A—C9A	160.60 (14)	O2B—S1B—C8B—C13B	153.64 (14)
O2A—S1A—C8A—C9A	30.26 (17)	O1B—S1B—C8B—C13B	22.98 (16)
N1A—S1A—C8A—C9A	−84.20 (16)	N1B—S1B—C8B—C13B	−91.29 (15)
C13A—C8A—C9A—C10A	−0.6 (3)	C13B—C8B—C9B—C10B	0.0 (3)
S1A—C8A—C9A—C10A	173.04 (14)	S1B—C8B—C9B—C10B	−178.61 (14)
C8A—C9A—C10A—C11A	0.0 (3)	C8B—C9B—C10B—C11B	0.0 (3)
C9A—C10A—C11A—C12A	1.1 (3)	C9B—C10B—C11B—C12B	0.1 (3)
C9A—C10A—C11A—C14A	−179.23 (18)	C9B—C10B—C11B—C14B	−178.65 (17)
C10A—C11A—C12A—C13A	−1.6 (3)	C10B—C11B—C12B—C13B	−0.4 (3)
C14A—C11A—C12A—C13A	178.73 (18)	C14B—C11B—C12B—C13B	178.44 (17)
C11A—C12A—C13A—C8A	1.0 (3)	C11B—C12B—C13B—C8B	0.4 (3)
C9A—C8A—C13A—C12A	0.1 (3)	C9B—C8B—C13B—C12B	−0.2 (3)
S1A—C8A—C13A—C12A	−173.60 (14)	S1B—C8B—C13B—C12B	178.40 (13)
C7A—C6A—C17A—C18A	178.10 (17)	O3B—C6B—C17B—C18B	−4.6 (2)
O3A—C6A—C17A—C18A	−2.8 (2)	C7B—C6B—C17B—C18B	174.79 (15)
C7A—C6A—C17A—C22A	−1.6 (2)	O3B—C6B—C17B—C22B	176.43 (14)
O3A—C6A—C17A—C22A	177.44 (15)	C7B—C6B—C17B—C22B	−4.1 (2)
C22A—C17A—C18A—C19A	−1.2 (3)	C22B—C17B—C18B—C19B	−1.1 (2)
C6A—C17A—C18A—C19A	179.03 (18)	C6B—C17B—C18B—C19B	180.00 (15)
C17A—C18A—C19A—C20A	−0.6 (3)	C17B—C18B—C19B—C20B	−1.1 (3)
C18A—C19A—C20A—C21A	1.3 (3)	C18B—C19B—C20B—C21B	1.6 (3)
C19A—C20A—C21A—C22A	−0.2 (3)	C19B—C20B—C21B—C22B	0.1 (3)
C23A—N2A—C22A—C21A	−178.97 (17)	C23B—N2B—C22B—C21B	179.33 (16)
C24A—N2A—C22A—C21A	−0.2 (3)	C24B—N2B—C22B—C21B	−1.4 (2)
C23A—N2A—C22A—C17A	−0.2 (3)	C23B—N2B—C22B—C17B	1.1 (2)
C24A—N2A—C22A—C17A	178.57 (16)	C24B—N2B—C22B—C17B	−179.57 (15)
C20A—C21A—C22A—N2A	177.11 (18)	C20B—C21B—C22B—N2B	179.46 (16)
C20A—C21A—C22A—C17A	−1.7 (3)	C20B—C21B—C22B—C17B	−2.3 (2)
C18A—C17A—C22A—N2A	−176.46 (16)	C18B—C17B—C22B—N2B	−178.97 (14)
C6A—C17A—C22A—N2A	3.3 (2)	C6B—C17B—C22B—N2B	0.0 (2)
C18A—C17A—C22A—C21A	2.4 (3)	C18B—C17B—C22B—C21B	2.8 (2)
C6A—C17A—C22A—C21A	−177.87 (16)	C6B—C17B—C22B—C21B	−178.24 (15)
C22A—N2A—C23A—O4A	177.08 (16)	C22B—N2B—C23B—O4B	−179.13 (16)
C24A—N2A—C23A—O4A	−1.7 (3)	C24B—N2B—C23B—O4B	1.6 (2)
C22A—N2A—C23A—C7A	−4.4 (2)	C22B—N2B—C23B—C7B	1.6 (2)
C24A—N2A—C23A—C7A	176.79 (16)	C24B—N2B—C23B—C7B	−177.71 (15)
C6A—C7A—C23A—O4A	−175.54 (17)	C6B—C7B—C23B—O4B	175.09 (16)
C3A—C7A—C23A—O4A	3.4 (3)	C3B—C7B—C23B—O4B	−2.9 (2)
C6A—C7A—C23A—N2A	6.0 (2)	C6B—C7B—C23B—N2B	−5.7 (2)
C3A—C7A—C23A—N2A	−175.02 (15)	C3B—C7B—C23B—N2B	176.38 (14)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1O···O2A^{i}	0.85 (3)	2.04 (3)	2.879 (3)	167 (3)
O1W—H2O···O4B	0.85 (3)	2.00 (3)	2.841 (2)	175 (4)

C2B—H2B···O1B^{ii}	0.98	2.59	3.485 (2)	152
C4A—H4A···N1A^{iii}	0.97	2.54	3.356 (2)	142
C4A—H4B···O4A	0.97	2.35	2.927 (2)	117
C4B—H4C···O4B	0.97	2.37	2.976 (2)	120
C14A—H14B···O1W^{iv}	0.96	2.57	3.521 (3)	170
C14B—H14F···O2B^{iv}	0.96	2.52	3.276 (3)	136
C15A—H15A···O1B	0.96	2.55	3.502 (2)	172
C16B—H16D···O4A^{i}	0.96	2.60	3.474 (2)	152
C12A—H12A···Cg1	0.93	2.87	3.684 (2)	147
C24A—H24C···Cg2^{v}	0.96	2.86	3.800 (2)	166

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

Fig. 1

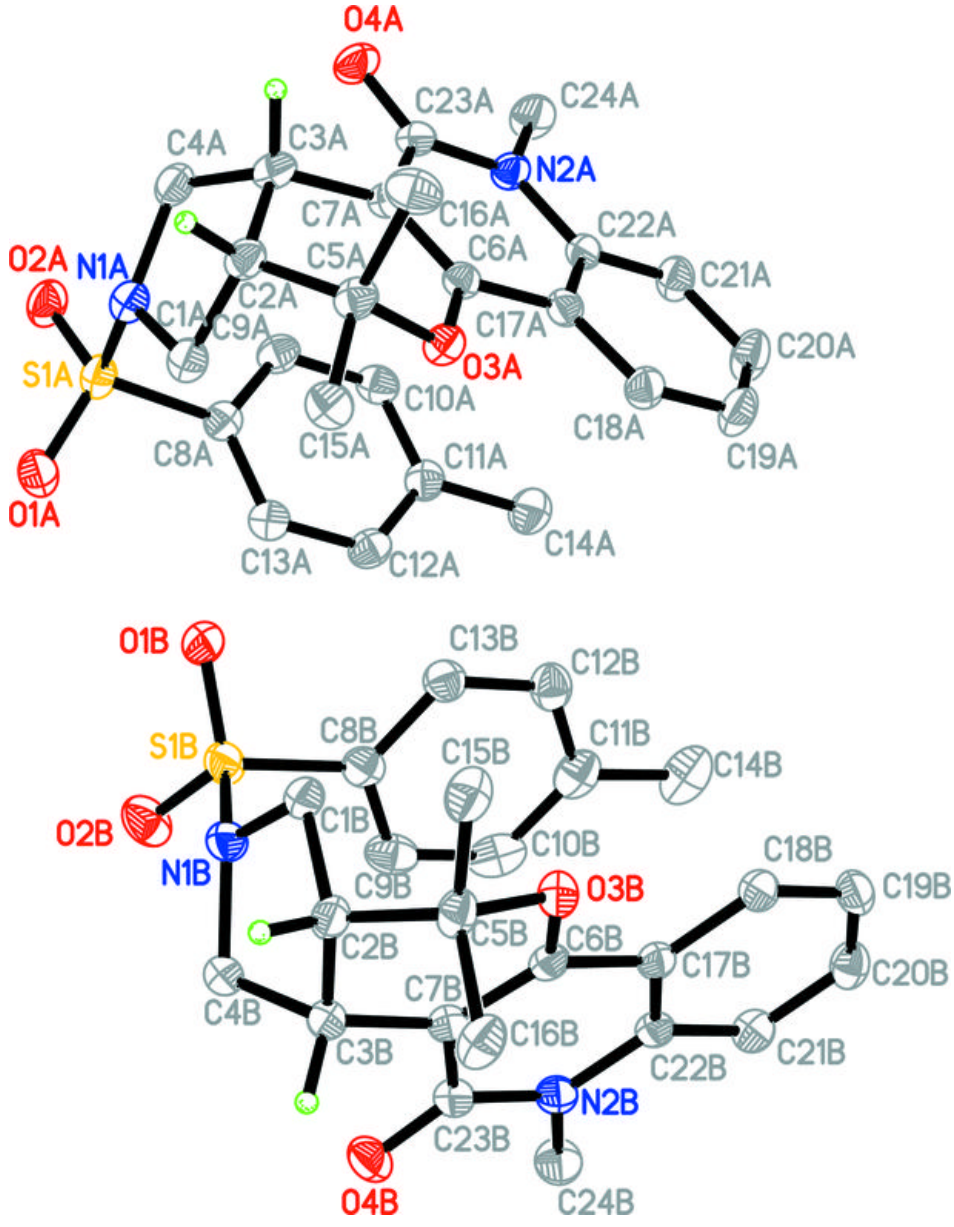

O4A
C23A
C24A
C4A
C3A
N2A
C7A
C16A
C22A
O2A
N1A
C5A
C6A
C21A
C1A
C2A
C9A
C17A
C20A
S1A
O3A
C10A
C18A
C8A
C15A
C11A
C19A
O1A
C14A
C13A
C12A
O1B
C13B
C12B
S1B
C8B
C15B
C11B
C14B
O2B
C1B
C10B
C18B
N1B
C9B
O3B
C19B
C2B
C5B
C6B
C17B
C20B
C7B
C4B
C16B
C3B
C22B
C21B
N2B
C23B
O4B
C24B

Fig. 2

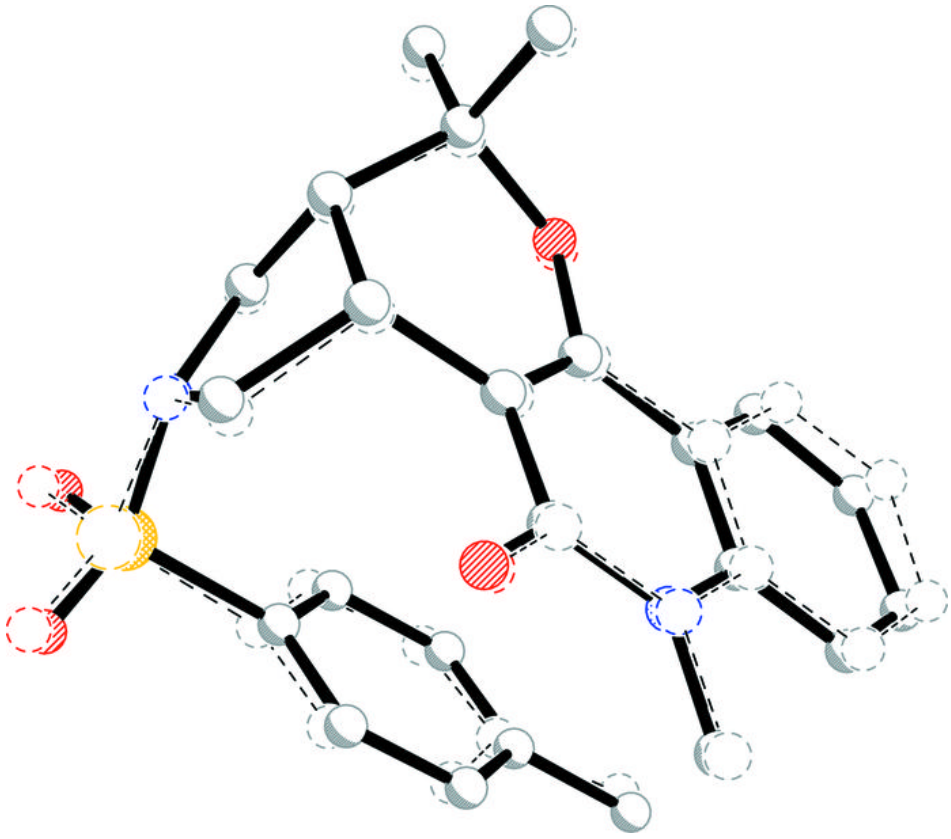


Fig. 3

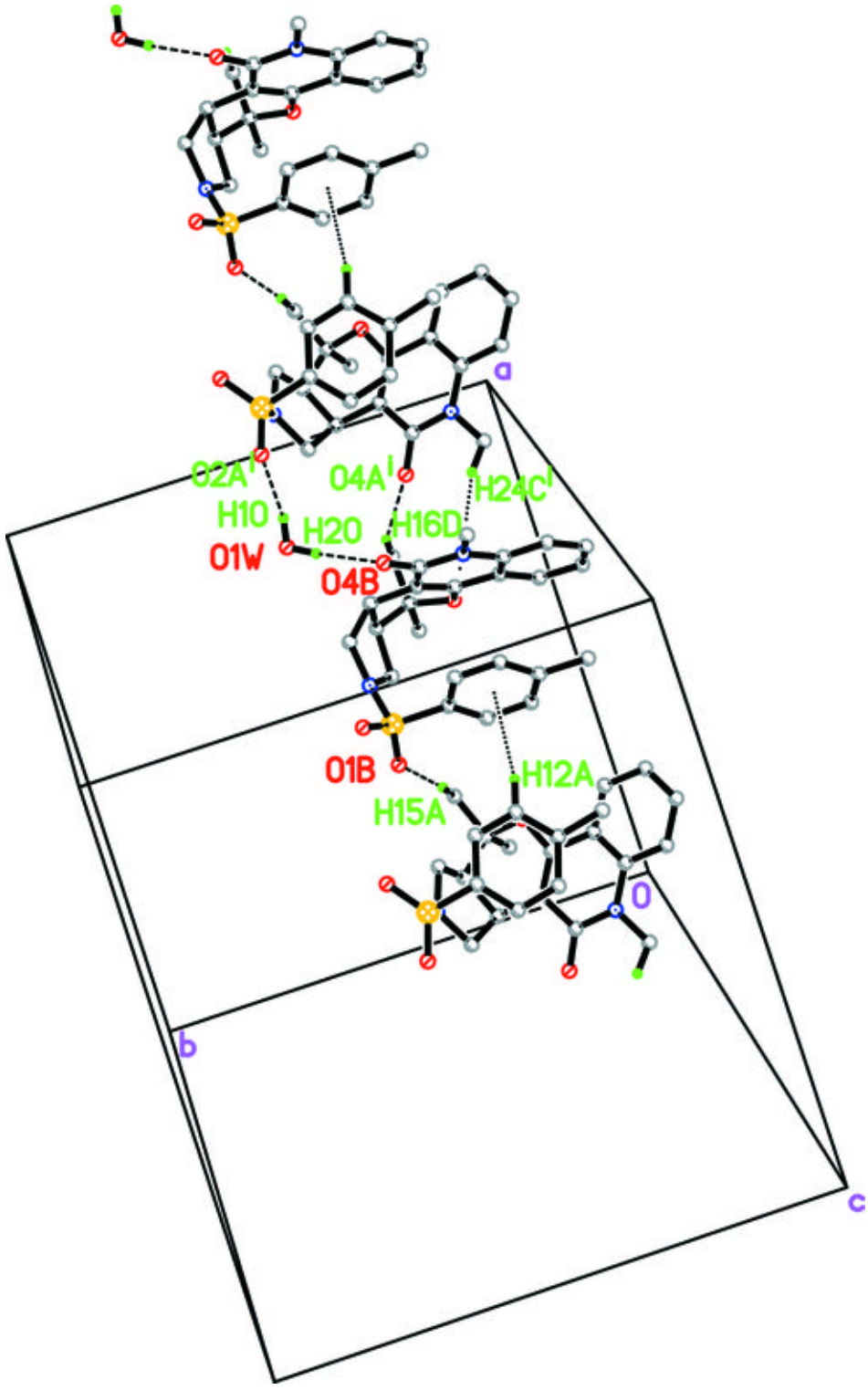
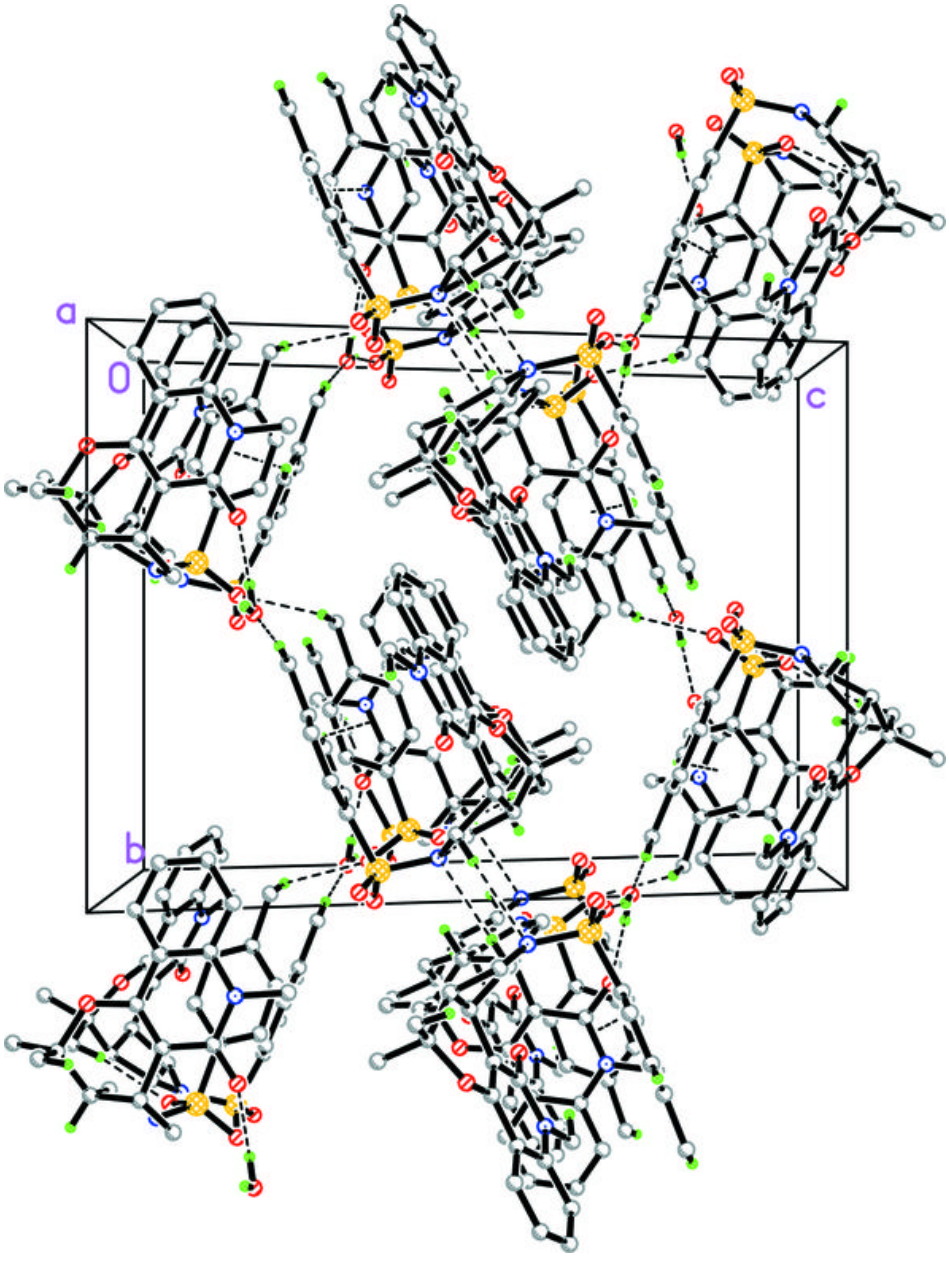


Fig. 4



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

K. Chinnakali,[a]* M. Jayagobi[b] and Hoong-Kun Fun[c]*

[a]Department of Physics, Anna University, Chennai 600 025, India, [b]Department of Organic Chemistry, University of Madras, Guindy Campus, Chennai 600 025, India, and [c]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia
Correspondence e-mail: kali@annauniv.edu, hkfun@usm.my

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.

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.

 doi:10.1107/S1600536807063817