Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4,4,7,7-Tetramethyl-2-tosyl-2,3,3a,4,-6,7,8,9-octahydro-1*H*-pyrrolo[3,4-*c*]-pyrano[6,5-*b*]cyclohexan-9-one

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

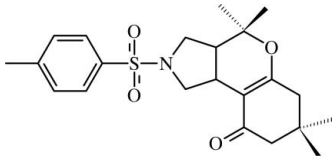
Received 18 October 2007; accepted 21 October 2007

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.046; wR factor = 0.128; data-to-parameter ratio = 26.7.

The title compound, $C_{22}H_{29}NO_4S$, crystallizes with three independent molecules, *A*, *B* and *C*, in the asymmetric unit. Each of the three independent molecules adopts a folded conformation, with the phenylsulfonyl group lying over the pyranocyclohexanone ring system, and with the pyrrolidine and dihydropyran rings *cis*-fused. In all three molecules, the pyrrolidine ring has a twist conformation and the dihydropyran ring is in a half-chair conformation. The cyclohexenone rings adopt envelope conformations, with the flap atom puckered towards the phenylsulfonyl group in molecule *A*, and away from that group in molecules *B* and *C*, resulting in a different overall conformation for molecule *A* compared to *B* and *C*. In all molecules, the tosyl group is equatorially attached to the pyrrolidine ring. In the crystal structure, the molecules are linked into a three-dimensional framework by C—H···O hydrogen bonds.

Related literature

For related pyrrolo[3,4-*c*]pyran structures, see: Chinnakali *et al.* (2007*a*,*b*). For biological activities of pyrrolo[3,4-*c*]pyran derivatives, see: Millan *et al.* (2000). For ring puckering parameters, see: Cremer & Pople (1975). For asymmetry parameters, see: Duax *et al.* (1976).



Experimental

Crystal data

$C_{22}H_{29}NO_4S$
M_r = 403.53
Triclinic, $P\overline{1}$
a = 14.5021 (7) Å
b = 15.0787 (7) Å
c = 16.9696 (8) Å
α = 64.059 (2)°
β = 69.821 (2)°
γ = 71.636 (3)°
V = 3072.3 (3) Å^3
Z = 6
Mo $K\alpha$ radiation
μ = 0.19 mm^{-1}
T = 100.0 (1) K
0.54 × 0.39 × 0.20 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.894, T_{max} = 0.963
64276 measured reflections
20257 independent reflections
15293 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.128
S = 1.06
20257 reflections
760 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2*A*—H2*A*···O1*C*	0.98	2.51	3.4447 (18)	160
C2*B*—H2*B*···O1*B*^{i}	0.98	2.52	3.4167 (18)	151
C2*C*—H2*C*···O1*A*	0.98	2.51	3.4739 (18)	167
C4*A*—H4*A*···O4*A*	0.97	2.48	2.9605 (17)	111
C4*B*—H4*C*···O4*B*	0.97	2.48	3.0370 (18)	116
C4*C*—H4*F*···O4*C*	0.97	2.43	3.0069 (17)	118
C12*A*—H12*A*···O2*C*^{ii}	0.93	2.51	3.2130 (16)	133
C12*B*—H12*B*···O2*A*^{iii}	0.93	2.59	3.3762 (18)	143
C14*C*—H14*I*···O2*C*^{iv}	0.96	2.56	3.362 (2)	142
C17*A*—H17*B*···O4*C*^{ii}	0.97	2.51	3.3480 (18)	145
C17*B*—H17*C*···O4*A*^{iii}	0.97	2.38	3.2776 (17)	154
C21*C*—H21*I*···O4*B*^{v}	0.96	2.47	3.3058 (17)	146
C22*A*—H22*B*···O4*C*^{ii}	0.96	2.55	3.4023 (16)	147

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2210).

References

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

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

  doi:10.1107/S1600536807052221

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.
Millan, M. J., Dekeyne, A., Rivet, J.-M., Dubuffet, T., Lavielle, G. & Brocco, M. (2000). *J. Pharmacol. Exp. Ther.* **293**, 1063–1073.
Sheldrick, G. M. (1998). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

supplementary materials

Acta Cryst. (2007). E**63**, o4436-o4437 [**doi:10.1107/S1600536807052221**]

4,4,7,7-Tetramethyl-2-tosyl-2,3,3a,4,6,7,8,9-octahydro-1*H*-pyrrolo[3,4-*c*]pyrano[6,5-*b*]cyclohexan-9-one

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

Comment

S33084, a pyrrolo[3,4-*c*]pyran derivative, is a novel, potent, selective, and competitive antagonist at dopamine D3-receptors (Millan *et al.*, 2000). Previously, we have reported the crystal structures of two pyrrolo[3,4-*c*]pyran derivatives (Chinnakali *et al.*, 2007*a*,b). Now we report here the crystal structure of the title compound.

The title compound crystallizes in space group $P\bar{1}$ with three independent molecules, A, B and C, in the asymmetric unit. The conformations of molecules B and C are the same but that of A is different. Views of the three independent molecules, with the atomic numbering schemes, are shown in Fig. 1. The weighted r.m.s. deviations for the superposition of the non-H atoms of any pair of molecules in the title compound using *XP* in *SHELXTL* (Sheldrick, 1998) are 0.675 (A/B pair), 0.629 (A/C pair) and 0.095 Å (B/C pair). Views of the superposition of molecular pairs are shown in Fig.2. The corresponding bond lengths and angles of the three molecules agree with each other and show normal values.

In all three molecules, the pyrrolidine ring (N1/C1—C4) adopts a twist conformation. In molecules B and C, the local twofold rotation axis passes through atom N1 and the mid-point of the opposite bond C2—C3, whereas in molecule A the axis passes through atom C4 and the C1—C2 bond. The puckering parameters (Cremer & Pople, 1975) for the pyrrolidine ring in A/B/C are q_2 = 0.395 (1)/0.359 (2)/0.362 (2) Å and φ = 54.9 (2)/86.0 (2)/267.2 (2)°. The smallest displacement asymmetry parameters (Duax *et al.*, 1976) are ΔC_2[C1A—C2A] = 1.0 (1)°, ΔC_2[C2B—C3B] = 4.4 (2)° and ΔC_2[C2C—C3C] = 3.2 (1)°. In each independent molecule, the N atom exhibits sp^3 hybridization and the tosyl group is equatorially attached to the pyrrolidine ring.

In each of the three independent molecules, the dihydropyran ring (O3/C5/C2/C3/C7/C6) 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/C are 0.432 (1)/0.462 (2)/0.459 (1) Å, 51.8 (2)/53.5 (2)/126.5 (2)°, 84.8 (2)/84.4 (2)/267.3 (2)° and 6.9 (2)/7.4 (2)/4.7 (2)°.

The cyclohexenone rings (C6/C7/C20/C19/C18/C17) in molecules A, B and C, adopt envelope conformations with atom C18 at the flap. The asymmetry parameter ΔC_S[C18] is 5.1 (2), 3.5 (2) and 1.1 (2)° for molecules A, B and C, respectively. The Q, θ and φ values for A/B/C are 0.460 (2)/0.452 (2)/0.438 (2) Å, 55.8 (2)/131.6 (2)/47.0 (2)° and 234.4 (2)/64.8 (2)/241.3 (3)°, respectively. The deviation of atom C18 from the C6/C7/C20/C19/C17 plane in molecule A [−0.641 (2) Å] is in the opposite direction to those in molecules B [0.627 (2) Å] and C [0.609 (2) Å]. This results in a different conformation for molecule A compared to B and C (Fig. 2).

Each of the three independent molecules adopt a folded conformation, with the phenylsulfonyl group lying over the pyranocyclohexanone ring system, and with the pyrrolidine and dihydropyran rings *cis*-fused.

Each of the independent molecules B and C forms a centrosymmetric dimer linked by paired C—H···O hydrogen bonds *viz*. C2B—H2B···O1B^{i} and C14C—H14I···O2C^{iv} (symmetry codes are given in Table 1). The B molecules form a dimer centred at (1/2,1/2,0), while the C molecules form a dimer centred at (0,1/2,1/2). The B and C dimers and A molecules are linked into a three-dimensional network by a number of C—H···O hydrogen bonds (Fig. 3).

Experimental

To a solution of 5,5-dimethylcyclohexane-1,3-dione (1 mmol) in dry toluene (20 ml), 2-[*N*-(3-methylbut-2-enyl)-*N*-tosylamino]acetaldehyde (1 mmol) and a catalytic amount of the base ethylenediamine-*N*,*N*'-diacetate (EDDA) were added and the reaction mixture was refluxed for 12 h. After completion of the reaction, the solvent was evaporated under reduced pressure and the crude product was chromatographed using a hexane-ethyl acetate (8:2 *v*/*v*) mixture to obtain the title compound. The compound was recrystallized from ethyl acetate solution by slow evaporation.

Refinement

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 attached to aromatic rings.

Figures

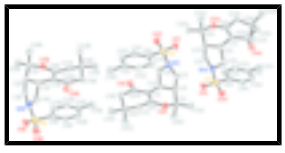


Fig. 1. The three independent molecules of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 80% probability level. H atoms have been omitted for clarity.

Fig. 2. Fit of (*a*) molecule A (dashed lines) on molecule B (solid lines), (*b*) molecule A (dashed lines) on molecule C (solid lines), and (*c*) molecule B (dashed lines) on molecule C (solid lines). H atoms have been omitted for clarity.

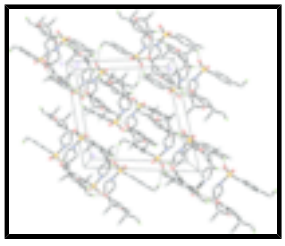


Fig. 3. View of the crystal packing of the title compound. Hydrogen bonds are shown as dashed lines. For the sake of clarity, H atoms not involved in the interactions have been omitted.

4,4,7,7-Tetramethyl-2-tosyl-2,3,3a,4,6,7,8,9-octahydro-1*H*- pyrrolo[3,4-*c*]pyrano[6,5-*b*]cyclohexan-9-one

Crystal data

$C_{22}H_{29}NO_4S$	$Z = 6$
$M_r = 403.53$	$F_{000} = 1296$
Triclinic, $P\overline{1}$	$D_x = 1.309$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å

a = 14.5021 (7) Å	Cell parameters from 6958 reflections
b = 15.0787 (7) Å	θ = 2.6–31.5º
c = 16.9696 (8) Å	μ = 0.19 mm^{-1}
α = 64.059 (2)º	T = 100.0 (1) K
β = 69.821 (2)º	Block, colourless
γ = 71.636 (3)º	0.54 × 0.39 × 0.20 mm
V = 3072.3 (3) $Å^3$	

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer	20257 independent reflections
Radiation source: fine-focus sealed tube	15293 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.042
Detector resolution: 8.33 pixels mm^{-1}	θ_{max} = 31.5º
T = 100.0(1) K	θ_{min} = 1.4º
ω scans	h = −21→21
Absorption correction: multi-scan (SADABS; Bruker, 2005)	k = −22→22
T_{min} = 0.894, T_{max} = 0.963	l = −24→24
64276 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
$R[F^2 > 2\sigma(F^2)]$ = 0.046	H-atom parameters constrained
$wR(F^2)$ = 0.128	$w = 1/[\sigma^2(F_o^2) + (0.0615P)^2 + 0.432P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.06	$(\Delta/\sigma)_{max}$ = 0.001
20257 reflections	$\Delta\rho_{max}$ = 0.44 e $Å^{-3}$
760 parameters	$\Delta\rho_{min}$ = −0.51 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 calculat-

ing *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	0.25730 (2)	0.00053 (2)	0.23582 (2)	0.01537 (7)
O1A	0.28101 (7)	−0.04754 (7)	0.32238 (7)	0.0219 (2)
O2A	0.33129 (7)	0.04251 (7)	0.15602 (7)	0.0210 (2)
O3A	−0.14661 (7)	0.12129 (7)	0.33197 (6)	0.01629 (18)
O4A	0.01788 (7)	0.21417 (7)	0.02177 (6)	0.01954 (19)
N1A	0.16405 (8)	0.09352 (8)	0.24168 (7)	0.0147 (2)
C1A	0.07741 (9)	0.07873 (9)	0.32023 (8)	0.0156 (2)
H1A	0.0958	0.0639	0.3752	0.019*
H1B	0.0470	0.0254	0.3286	0.019*
C2A	0.00837 (9)	0.18133 (9)	0.29219 (8)	0.0140 (2)
H2A	0.0351	0.2296	0.2982	0.017*
C3A	0.02031 (9)	0.20865 (9)	0.19085 (8)	0.0136 (2)
H3A	0.0098	0.2819	0.1597	0.016*
C4A	0.13049 (9)	0.16124 (9)	0.15738 (8)	0.0161 (2)
H4A	0.1349	0.1235	0.1219	0.019*
H4B	0.1708	0.2126	0.1210	0.019*
C5A	−0.10039 (9)	0.18450 (9)	0.34712 (8)	0.0151 (2)
C6A	−0.12884 (9)	0.12720 (9)	0.24667 (8)	0.0140 (2)
C7A	−0.05380 (9)	0.16780 (9)	0.17777 (8)	0.0139 (2)
C8A	0.21535 (9)	−0.08592 (9)	0.21879 (8)	0.0151 (2)
C9A	0.23804 (9)	−0.08690 (10)	0.13255 (9)	0.0169 (2)
H9A	0.2754	−0.0423	0.0838	0.020*
C10A	0.20415 (10)	−0.15542 (10)	0.12004 (9)	0.0182 (2)
H10A	0.2205	−0.1573	0.0627	0.022*
C11A	0.14599 (9)	−0.22137 (9)	0.19239 (9)	0.0176 (2)
C12A	0.12421 (10)	−0.21869 (10)	0.27782 (9)	0.0195 (3)
H12A	0.0856	−0.2623	0.3264	0.023*
C13A	0.15886 (10)	−0.15229 (9)	0.29224 (9)	0.0180 (2)
H13A	0.1446	−0.1521	0.3500	0.022*
C14A	0.10751 (11)	−0.29328 (10)	0.17736 (10)	0.0237 (3)
H14A	0.0789	−0.3401	0.2346	0.036*
H14B	0.1618	−0.3292	0.1443	0.036*
H14C	0.0573	−0.2563	0.1436	0.036*
C15A	−0.10928 (10)	0.13859 (10)	0.44833 (9)	0.0196 (3)
H15A	−0.1787	0.1423	0.4798	0.029*
H15B	−0.0793	0.1749	0.4642	0.029*
H15C	−0.0754	0.0695	0.4649	0.029*
C16A	−0.16078 (10)	0.29122 (10)	0.31870 (9)	0.0203 (3)
H16A	−0.2288	0.2916	0.3539	0.030*
H16B	−0.1596	0.3155	0.2558	0.030*
H16C	−0.1322	0.3339	0.3284	0.030*
C17A	−0.20253 (9)	0.08353 (10)	0.23786 (8)	0.0170 (2)

H17A	−0.2640	0.1332	0.2319	0.020*
H17B	−0.2181	0.0260	0.2927	0.020*
C18A	−0.16466 (9)	0.05037 (10)	0.15700 (8)	0.0162 (2)
C19A	−0.12275 (10)	0.13658 (10)	0.07437 (8)	0.0174 (2)
H19A	−0.0921	0.1141	0.0239	0.021*
H19B	−0.1779	0.1920	0.0585	0.021*
C20A	−0.04644 (9)	0.17479 (9)	0.08724 (8)	0.0150 (2)
C21A	−0.08307 (10)	−0.04498 (10)	0.17470 (10)	0.0224 (3)
H21A	−0.0600	−0.0649	0.1235	0.034*
H21B	−0.1101	−0.0980	0.2274	0.034*
H21C	−0.0281	−0.0317	0.1843	0.034*
C22A	−0.25169 (10)	0.02860 (11)	0.14144 (9)	0.0219 (3)
H22A	−0.3030	0.0881	0.1303	0.033*
H22B	−0.2785	−0.0246	0.1940	0.033*
H22C	−0.2282	0.0087	0.0902	0.033*
S1B	0.58153 (2)	0.36735 (2)	0.91676 (2)	0.01783 (7)
O1B	0.60377 (7)	0.31500 (7)	1.00416 (7)	0.0230 (2)
O2B	0.65469 (7)	0.41543 (8)	0.83988 (7)	0.0246 (2)
O3B	0.20929 (7)	0.39100 (7)	1.00821 (6)	0.01585 (18)
O4B	0.36565 (7)	0.53637 (7)	0.69990 (6)	0.0212 (2)
N1B	0.48350 (8)	0.45447 (8)	0.92689 (7)	0.0166 (2)
C1B	0.39849 (9)	0.42918 (10)	1.00667 (8)	0.0169 (2)
H1C	0.4102	0.4313	1.0587	0.020*
H1D	0.3872	0.3630	1.0217	0.020*
C2B	0.30988 (10)	0.51128 (9)	0.97598 (8)	0.0163 (2)
H2B	0.3087	0.5707	0.9864	0.020*
C3B	0.33392 (9)	0.53689 (9)	0.87399 (8)	0.0152 (2)
H3B	0.3009	0.6059	0.8442	0.018*
C4B	0.44818 (10)	0.52853 (10)	0.84526 (9)	0.0183 (2)
H4C	0.4776	0.5050	0.7954	0.022*
H4D	0.4654	0.5930	0.8271	0.022*
C5B	0.20938 (10)	0.47821 (9)	1.02573 (8)	0.0164 (2)
C6B	0.24455 (9)	0.39631 (9)	0.92183 (8)	0.0133 (2)
C7B	0.30000 (9)	0.46398 (9)	0.85579 (8)	0.0136 (2)
C8B	0.54718 (9)	0.28174 (9)	0.89251 (9)	0.0166 (2)
C9B	0.56429 (10)	0.29192 (10)	0.80321 (9)	0.0193 (3)
H9B	0.5958	0.3426	0.7562	0.023*
C10B	0.53371 (10)	0.22542 (10)	0.78513 (9)	0.0208 (3)
H10B	0.5458	0.2315	0.7257	0.025*
C11B	0.48518 (10)	0.14986 (10)	0.85493 (10)	0.0201 (3)
C12B	0.46883 (10)	0.14092 (10)	0.94360 (10)	0.0203 (3)
H12B	0.4363	0.0910	0.9906	0.024*
C13B	0.50051 (10)	0.20558 (10)	0.96285 (9)	0.0187 (2)
H13B	0.4905	0.1980	1.0225	0.022*
C14B	0.44979 (11)	0.07989 (11)	0.83458 (12)	0.0293 (3)
H14D	0.4512	0.0158	0.8836	0.044*
H14E	0.4930	0.0714	0.7799	0.044*
H14F	0.3826	0.1080	0.8273	0.044*
C15B	0.19143 (11)	0.44044 (11)	1.12761 (9)	0.0218 (3)

H15D	0.1275	0.4206	1.1557	0.033*
H15E	0.1923	0.4931	1.1446	0.033*
H15F	0.2431	0.3838	1.1470	0.033*
C16B	0.12321 (10)	0.56104 (10)	0.99339 (9)	0.0223 (3)
H16D	0.0612	0.5379	1.0259	0.033*
H16E	0.1324	0.5783	0.9300	0.033*
H16F	0.1216	0.6192	1.0039	0.033*
C17B	0.21490 (9)	0.31860 (9)	0.90774 (8)	0.0154 (2)
H17C	0.1542	0.3003	0.9528	0.018*
H17D	0.2672	0.2588	0.9160	0.018*
C18B	0.19713 (9)	0.35647 (9)	0.81308 (8)	0.0145 (2)
C19B	0.28960 (9)	0.39721 (10)	0.74443 (8)	0.0167 (2)
H19C	0.3450	0.3409	0.7431	0.020*
H19D	0.2759	0.4297	0.6850	0.020*
C20B	0.32205 (9)	0.47148 (9)	0.76271 (8)	0.0153 (2)
C21B	0.18315 (10)	0.26915 (10)	0.79817 (9)	0.0200 (3)
H21D	0.1720	0.2925	0.7391	0.030*
H21E	0.1265	0.2428	0.8430	0.030*
H21F	0.2421	0.2173	0.8031	0.030*
C22B	0.10247 (9)	0.43823 (10)	0.80570 (9)	0.0185 (2)
H22D	0.0914	0.4618	0.7466	0.028*
H22E	0.1104	0.4931	0.8156	0.028*
H22F	0.0461	0.4111	0.8503	0.028*
S1C	0.06942 (2)	0.31075 (2)	0.43203 (2)	0.01595 (7)
O1C	0.04312 (7)	0.36155 (7)	0.34654 (6)	0.0209 (2)
O2C	−0.00541 (7)	0.27458 (7)	0.51339 (6)	0.0217 (2)
O3C	0.44398 (7)	0.23966 (7)	0.32573 (6)	0.01574 (18)
O4C	0.29178 (7)	0.12901 (7)	0.63807 (6)	0.01970 (19)
N1C	0.15528 (8)	0.21312 (8)	0.42480 (7)	0.0153 (2)
C1C	0.23803 (9)	0.22488 (10)	0.34229 (8)	0.0162 (2)
H1E	0.2597	0.2878	0.3211	0.019*
H1F	0.2179	0.2227	0.2944	0.019*
C2C	0.32110 (9)	0.13502 (9)	0.37290 (8)	0.0144 (2)
H2C	0.3104	0.0764	0.3686	0.017*
C3C	0.30547 (9)	0.11588 (9)	0.47298 (8)	0.0142 (2)
H3C	0.3327	0.0455	0.5055	0.017*
C4C	0.19076 (9)	0.13798 (9)	0.50623 (8)	0.0165 (2)
H4E	0.1641	0.0774	0.5297	0.020*
H4F	0.1706	0.1652	0.5533	0.020*
C5C	0.42593 (9)	0.15428 (9)	0.31662 (8)	0.0155 (2)
C6C	0.41611 (9)	0.24271 (9)	0.40928 (8)	0.0137 (2)
C7C	0.35476 (9)	0.18503 (9)	0.48107 (8)	0.0132 (2)
C8C	0.12120 (9)	0.39334 (9)	0.44529 (8)	0.0156 (2)
C9C	0.10565 (10)	0.39398 (10)	0.53056 (9)	0.0190 (3)
H9C	0.0693	0.3500	0.5811	0.023*
C10C	0.14503 (10)	0.46115 (10)	0.53951 (9)	0.0206 (3)
H10C	0.1336	0.4626	0.5964	0.025*
C11C	0.20147 (10)	0.52656 (10)	0.46448 (9)	0.0188 (3)
C12C	0.21710 (10)	0.52384 (10)	0.37981 (9)	0.0200 (3)

H12C	0.2553	0.5663	0.3295	0.024*
C13C	0.17642 (10)	0.45861 (10)	0.36939 (9)	0.0189 (3)
H13C	0.1860	0.4586	0.3123	0.023*
C14C	0.24354 (11)	0.59926 (11)	0.47523 (11)	0.0255 (3)
H14G	0.2928	0.6262	0.4212	0.038*
H14H	0.2741	0.5647	0.5255	0.038*
H14I	0.1905	0.6530	0.4859	0.038*
C15C	0.43654 (10)	0.18716 (10)	0.21621 (8)	0.0192 (3)
H15G	0.5033	0.1983	0.1838	0.029*
H15H	0.3893	0.2483	0.1965	0.029*
H15I	0.4237	0.1357	0.2048	0.029*
C16C	0.50641 (10)	0.06369 (10)	0.34852 (9)	0.0208 (3)
H16G	0.5711	0.0781	0.3120	0.031*
H16H	0.4962	0.0068	0.3433	0.031*
H16I	0.5028	0.0489	0.4105	0.031*
C17C	0.45921 (10)	0.31889 (9)	0.41250 (8)	0.0166 (2)
H17E	0.4135	0.3833	0.3981	0.020*
H17F	0.5219	0.3265	0.3670	0.020*
C18C	0.47790 (9)	0.28933 (10)	0.50539 (8)	0.0159 (2)
C19C	0.38213 (10)	0.26125 (10)	0.57732 (8)	0.0173 (2)
H19E	0.3961	0.2337	0.6364	0.021*
H19F	0.3316	0.3221	0.5736	0.021*
C20C	0.33934 (9)	0.18652 (9)	0.57013 (8)	0.0143 (2)
C21C	0.50086 (11)	0.37855 (11)	0.51048 (9)	0.0239 (3)
H21G	0.5125	0.3597	0.5686	0.036*
H21H	0.4451	0.4339	0.5018	0.036*
H21I	0.5595	0.3982	0.4642	0.036*
C22C	0.56620 (10)	0.20100 (11)	0.52004 (10)	0.0234 (3)
H22G	0.5776	0.1828	0.5781	0.035*
H22H	0.6250	0.2200	0.4738	0.035*
H22I	0.5514	0.1447	0.5174	0.035*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1A	0.01382 (13)	0.01656 (14)	0.01820 (15)	−0.00132 (11)	−0.00606 (11)	−0.00806 (12)
O1A	0.0239 (5)	0.0223 (5)	0.0238 (5)	0.0022 (4)	−0.0147 (4)	−0.0102 (4)
O2A	0.0147 (4)	0.0244 (5)	0.0255 (5)	−0.0060 (4)	−0.0017 (4)	−0.0116 (4)
O3A	0.0179 (4)	0.0197 (4)	0.0136 (4)	−0.0086 (3)	−0.0012 (3)	−0.0069 (3)
O4A	0.0192 (4)	0.0243 (5)	0.0141 (4)	−0.0104 (4)	−0.0021 (4)	−0.0034 (4)
N1A	0.0151 (5)	0.0153 (5)	0.0128 (5)	−0.0018 (4)	−0.0043 (4)	−0.0046 (4)
C1A	0.0155 (5)	0.0159 (5)	0.0142 (5)	−0.0023 (4)	−0.0040 (4)	−0.0046 (4)
C2A	0.0148 (5)	0.0144 (5)	0.0142 (5)	−0.0038 (4)	−0.0037 (4)	−0.0059 (4)
C3A	0.0138 (5)	0.0129 (5)	0.0142 (5)	−0.0041 (4)	−0.0038 (4)	−0.0038 (4)
C4A	0.0149 (5)	0.0175 (6)	0.0135 (5)	−0.0043 (4)	−0.0036 (4)	−0.0025 (5)
C5A	0.0161 (5)	0.0163 (5)	0.0146 (5)	−0.0047 (4)	−0.0035 (4)	−0.0066 (5)
C6A	0.0151 (5)	0.0138 (5)	0.0131 (5)	−0.0041 (4)	−0.0038 (4)	−0.0038 (4)
C7A	0.0145 (5)	0.0140 (5)	0.0134 (5)	−0.0047 (4)	−0.0038 (4)	−0.0036 (4)

C8A	0.0159 (5)	0.0143 (5)	0.0158 (6)	−0.0016 (4)	−0.0049 (5)	−0.0064 (5)
C9A	0.0177 (6)	0.0183 (6)	0.0149 (6)	−0.0037 (5)	−0.0035 (5)	−0.0065 (5)
C10A	0.0194 (6)	0.0217 (6)	0.0162 (6)	−0.0032 (5)	−0.0061 (5)	−0.0085 (5)
C11A	0.0164 (5)	0.0161 (6)	0.0228 (6)	−0.0009 (5)	−0.0082 (5)	−0.0084 (5)
C12A	0.0203 (6)	0.0156 (6)	0.0191 (6)	−0.0045 (5)	−0.0035 (5)	−0.0038 (5)
C13A	0.0212 (6)	0.0161 (6)	0.0155 (6)	−0.0023 (5)	−0.0038 (5)	−0.0061 (5)
C14A	0.0241 (7)	0.0205 (6)	0.0322 (8)	−0.0054 (5)	−0.0114 (6)	−0.0105 (6)
C15A	0.0218 (6)	0.0234 (6)	0.0156 (6)	−0.0070 (5)	−0.0031 (5)	−0.0084 (5)
C16A	0.0173 (6)	0.0183 (6)	0.0236 (6)	−0.0019 (5)	−0.0026 (5)	−0.0093 (5)
C17A	0.0166 (5)	0.0200 (6)	0.0155 (6)	−0.0096 (5)	−0.0026 (5)	−0.0044 (5)
C18A	0.0176 (6)	0.0185 (6)	0.0152 (6)	−0.0083 (5)	−0.0041 (5)	−0.0052 (5)
C19A	0.0189 (6)	0.0214 (6)	0.0141 (5)	−0.0089 (5)	−0.0047 (5)	−0.0043 (5)
C20A	0.0153 (5)	0.0143 (5)	0.0146 (5)	−0.0043 (4)	−0.0042 (4)	−0.0031 (4)
C21A	0.0251 (7)	0.0198 (6)	0.0249 (7)	−0.0053 (5)	−0.0068 (6)	−0.0092 (5)
C22A	0.0237 (6)	0.0266 (7)	0.0189 (6)	−0.0137 (5)	−0.0050 (5)	−0.0057 (5)
S1B	0.01645 (14)	0.01895 (15)	0.02195 (16)	−0.00511 (11)	−0.00590 (12)	−0.00887 (12)
O1B	0.0247 (5)	0.0235 (5)	0.0275 (5)	−0.0022 (4)	−0.0141 (4)	−0.0110 (4)
O2B	0.0188 (5)	0.0263 (5)	0.0306 (5)	−0.0095 (4)	−0.0023 (4)	−0.0114 (4)
O3B	0.0200 (4)	0.0178 (4)	0.0106 (4)	−0.0076 (3)	−0.0006 (3)	−0.0056 (3)
O4B	0.0231 (5)	0.0246 (5)	0.0133 (4)	−0.0128 (4)	0.0007 (4)	−0.0031 (4)
N1B	0.0179 (5)	0.0164 (5)	0.0174 (5)	−0.0054 (4)	−0.0049 (4)	−0.0061 (4)
C1B	0.0187 (6)	0.0178 (6)	0.0160 (6)	−0.0042 (5)	−0.0051 (5)	−0.0066 (5)
C2B	0.0209 (6)	0.0140 (5)	0.0165 (6)	−0.0039 (5)	−0.0051 (5)	−0.0072 (5)
C3B	0.0179 (6)	0.0128 (5)	0.0153 (5)	−0.0051 (4)	−0.0044 (5)	−0.0039 (4)
C4B	0.0191 (6)	0.0180 (6)	0.0184 (6)	−0.0085 (5)	−0.0054 (5)	−0.0031 (5)
C5B	0.0199 (6)	0.0158 (5)	0.0142 (5)	−0.0032 (5)	−0.0031 (5)	−0.0072 (5)
C6B	0.0129 (5)	0.0150 (5)	0.0120 (5)	−0.0030 (4)	−0.0031 (4)	−0.0046 (4)
C7B	0.0143 (5)	0.0144 (5)	0.0130 (5)	−0.0046 (4)	−0.0027 (4)	−0.0049 (4)
C8B	0.0154 (5)	0.0165 (6)	0.0196 (6)	−0.0032 (4)	−0.0047 (5)	−0.0077 (5)
C9B	0.0186 (6)	0.0197 (6)	0.0184 (6)	−0.0050 (5)	−0.0029 (5)	−0.0065 (5)
C10B	0.0218 (6)	0.0229 (6)	0.0215 (6)	−0.0008 (5)	−0.0088 (5)	−0.0114 (5)
C11B	0.0155 (6)	0.0172 (6)	0.0315 (7)	0.0013 (5)	−0.0099 (5)	−0.0123 (5)
C12B	0.0179 (6)	0.0161 (6)	0.0261 (7)	−0.0041 (5)	−0.0033 (5)	−0.0081 (5)
C13B	0.0199 (6)	0.0179 (6)	0.0177 (6)	−0.0032 (5)	−0.0033 (5)	−0.0075 (5)
C14B	0.0260 (7)	0.0253 (7)	0.0487 (10)	0.0002 (6)	−0.0200 (7)	−0.0197 (7)
C15B	0.0270 (7)	0.0238 (7)	0.0144 (6)	−0.0035 (5)	−0.0034 (5)	−0.0091 (5)
C16B	0.0211 (6)	0.0215 (6)	0.0196 (6)	0.0013 (5)	−0.0034 (5)	−0.0082 (5)
C17B	0.0168 (5)	0.0153 (5)	0.0149 (5)	−0.0072 (4)	−0.0037 (5)	−0.0036 (4)
C18B	0.0148 (5)	0.0170 (5)	0.0136 (5)	−0.0049 (4)	−0.0028 (4)	−0.0067 (5)
C19B	0.0167 (5)	0.0221 (6)	0.0135 (5)	−0.0055 (5)	−0.0014 (5)	−0.0091 (5)
C20B	0.0134 (5)	0.0168 (5)	0.0142 (5)	−0.0037 (4)	−0.0020 (4)	−0.0049 (5)
C21B	0.0208 (6)	0.0225 (6)	0.0221 (6)	−0.0083 (5)	−0.0038 (5)	−0.0111 (5)
C22B	0.0155 (5)	0.0219 (6)	0.0195 (6)	−0.0020 (5)	−0.0046 (5)	−0.0097 (5)
S1C	0.01428 (13)	0.01932 (15)	0.01696 (14)	−0.00348 (11)	−0.00379 (11)	−0.00892 (12)
O1C	0.0216 (5)	0.0231 (5)	0.0218 (5)	0.0004 (4)	−0.0114 (4)	−0.0104 (4)
O2C	0.0168 (4)	0.0272 (5)	0.0227 (5)	−0.0079 (4)	0.0010 (4)	−0.0127 (4)
O3C	0.0195 (4)	0.0173 (4)	0.0121 (4)	−0.0082 (3)	−0.0012 (3)	−0.0057 (3)
O4C	0.0236 (5)	0.0216 (5)	0.0130 (4)	−0.0115 (4)	−0.0015 (4)	−0.0029 (4)
N1C	0.0144 (5)	0.0179 (5)	0.0139 (5)	−0.0031 (4)	−0.0028 (4)	−0.0066 (4)

C1C	0.0168 (5)	0.0184 (6)	0.0134 (5)	−0.0032 (5)	−0.0033 (4)	−0.0063 (5)
C2C	0.0160 (5)	0.0141 (5)	0.0149 (5)	−0.0043 (4)	−0.0036 (4)	−0.0063 (4)
C3C	0.0163 (5)	0.0133 (5)	0.0128 (5)	−0.0053 (4)	−0.0029 (4)	−0.0035 (4)
C4C	0.0167 (5)	0.0171 (6)	0.0149 (6)	−0.0071 (5)	−0.0034 (5)	−0.0031 (5)
C5C	0.0169 (5)	0.0154 (5)	0.0155 (6)	−0.0043 (4)	−0.0024 (5)	−0.0074 (5)
C6C	0.0147 (5)	0.0153 (5)	0.0119 (5)	−0.0043 (4)	−0.0041 (4)	−0.0042 (4)
C7C	0.0139 (5)	0.0136 (5)	0.0131 (5)	−0.0045 (4)	−0.0031 (4)	−0.0048 (4)
C8C	0.0157 (5)	0.0162 (6)	0.0163 (6)	−0.0018 (4)	−0.0044 (5)	−0.0076 (5)
C9C	0.0206 (6)	0.0223 (6)	0.0147 (6)	−0.0069 (5)	−0.0016 (5)	−0.0074 (5)
C10C	0.0241 (6)	0.0250 (7)	0.0164 (6)	−0.0048 (5)	−0.0069 (5)	−0.0095 (5)
C11C	0.0185 (6)	0.0170 (6)	0.0237 (6)	−0.0004 (5)	−0.0093 (5)	−0.0088 (5)
C12C	0.0200 (6)	0.0160 (6)	0.0211 (6)	−0.0045 (5)	−0.0022 (5)	−0.0056 (5)
C13C	0.0242 (6)	0.0180 (6)	0.0143 (6)	−0.0045 (5)	−0.0038 (5)	−0.0061 (5)
C14C	0.0247 (7)	0.0224 (7)	0.0347 (8)	−0.0055 (5)	−0.0108 (6)	−0.0118 (6)
C15C	0.0224 (6)	0.0226 (6)	0.0138 (6)	−0.0064 (5)	−0.0019 (5)	−0.0081 (5)
C16C	0.0176 (6)	0.0214 (6)	0.0206 (6)	−0.0008 (5)	−0.0032 (5)	−0.0083 (5)
C17C	0.0200 (6)	0.0167 (6)	0.0141 (5)	−0.0089 (5)	−0.0039 (5)	−0.0030 (5)
C18C	0.0175 (5)	0.0190 (6)	0.0137 (5)	−0.0087 (5)	−0.0036 (5)	−0.0048 (5)
C19C	0.0192 (6)	0.0210 (6)	0.0146 (6)	−0.0086 (5)	−0.0015 (5)	−0.0078 (5)
C20C	0.0134 (5)	0.0151 (5)	0.0139 (5)	−0.0041 (4)	−0.0023 (4)	−0.0047 (4)
C21C	0.0305 (7)	0.0292 (7)	0.0180 (6)	−0.0184 (6)	−0.0036 (5)	−0.0072 (6)
C22C	0.0188 (6)	0.0283 (7)	0.0215 (6)	−0.0066 (5)	−0.0065 (5)	−0.0051 (6)

Geometric parameters (Å, °)

S1A—O1A	1.4356 (10)	C10B—H10B	0.93
S1A—O2A	1.4358 (10)	C11B—C12B	1.391 (2)
S1A—N1A	1.6245 (11)	C11B—C14B	1.5094 (19)
S1A—C8A	1.7617 (13)	C12B—C13B	1.3903 (19)
O3A—C6A	1.3468 (14)	C12B—H12B	0.93
O3A—C5A	1.4696 (15)	C13B—H13B	0.93
O4A—C20A	1.2305 (14)	C14B—H14D	0.96
N1A—C1A	1.4718 (15)	C14B—H14E	0.96
N1A—C4A	1.4883 (15)	C14B—H14F	0.96
C1A—C2A	1.5267 (17)	C15B—H15D	0.96
C1A—H1A	0.97	C15B—H15E	0.96
C1A—H1B	0.97	C15B—H15F	0.96
C2A—C5A	1.5284 (17)	C16B—H16D	0.96
C2A—C3A	1.5416 (17)	C16B—H16E	0.96
C2A—H2A	0.98	C16B—H16F	0.96
C3A—C7A	1.5115 (17)	C17B—C18B	1.5371 (17)
C3A—C4A	1.5479 (17)	C17B—H17C	0.97
C3A—H3A	0.98	C17B—H17D	0.97
C4A—H4A	0.97	C18B—C21B	1.5277 (18)
C4A—H4B	0.97	C18B—C22B	1.5289 (17)
C5A—C15A	1.5195 (17)	C18B—C19B	1.5324 (17)
C5A—C16A	1.5210 (18)	C19B—C20B	1.5194 (18)
C6A—C7A	1.3571 (16)	C19B—H19C	0.97
C6A—C17A	1.4960 (17)	C19B—H19D	0.97

C7A—C20A	1.4611 (17)	C21B—H21D	0.96
C8A—C9A	1.3907 (18)	C21B—H21E	0.96
C8A—C13A	1.3953 (17)	C21B—H21F	0.96
C9A—C10A	1.3920 (18)	C22B—H22D	0.96
C9A—H9A	0.93	C22B—H22E	0.96
C10A—C11A	1.3977 (18)	C22B—H22F	0.96
C10A—H10A	0.93	S1C—O2C	1.4358 (10)
C11A—C12A	1.3895 (19)	S1C—O1C	1.4360 (10)
C11A—C14A	1.5078 (18)	S1C—N1C	1.6219 (11)
C12A—C13A	1.3896 (19)	S1C—C8C	1.7652 (13)
C12A—H12A	0.93	O3C—C6C	1.3511 (14)
C13A—H13A	0.93	O3C—C5C	1.4712 (15)
C14A—H14A	0.96	O4C—C20C	1.2290 (14)
C14A—H14B	0.96	N1C—C1C	1.4798 (16)
C14A—H14C	0.96	N1C—C4C	1.4871 (16)
C15A—H15A	0.96	C1C—C2C	1.5311 (17)
C15A—H15B	0.96	C1C—H1E	0.97
C15A—H15C	0.96	C1C—H1F	0.97
C16A—H16A	0.96	C2C—C5C	1.5302 (17)
C16A—H16B	0.96	C2C—C3C	1.5382 (17)
C16A—H16C	0.96	C2C—H2C	0.98
C17A—C18A	1.5303 (18)	C3C—C7C	1.5098 (17)
C17A—H17A	0.97	C3C—C4C	1.5377 (17)
C17A—H17B	0.97	C3C—H3C	0.98
C18A—C22A	1.5288 (18)	C4C—H4E	0.97
C18A—C19A	1.5299 (17)	C4C—H4F	0.97
C18A—C21A	1.5339 (18)	C5C—C15C	1.5169 (17)
C19A—C20A	1.5108 (17)	C5C—C16C	1.5185 (18)
C19A—H19A	0.97	C6C—C7C	1.3583 (16)
C19A—H19B	0.97	C6C—C17C	1.4981 (17)
C21A—H21A	0.96	C7C—C20C	1.4587 (17)
C21A—H21B	0.96	C8C—C9C	1.3894 (18)
C21A—H21C	0.96	C8C—C13C	1.3946 (17)
C22A—H22A	0.96	C9C—C10C	1.3906 (19)
C22A—H22B	0.96	C9C—H9C	0.93
C22A—H22C	0.96	C10C—C11C	1.3982 (19)
S1B—O2B	1.4337 (10)	C10C—H10C	0.93
S1B—O1B	1.4395 (10)	C11C—C12C	1.3923 (19)
S1B—N1B	1.6212 (11)	C11C—C14C	1.5102 (19)
S1B—C8B	1.7592 (13)	C12C—C13C	1.3916 (19)
O3B—C6B	1.3500 (14)	C12C—H12C	0.93
O3B—C5B	1.4701 (15)	C13C—H13C	0.93
O4B—C20B	1.2271 (15)	C14C—H14G	0.96
N1B—C1B	1.4803 (16)	C14C—H14H	0.96
N1B—C4B	1.4846 (16)	C14C—H14I	0.96
C1B—C2B	1.5331 (17)	C15C—H15G	0.96
C1B—H1C	0.97	C15C—H15H	0.96
C1B—H1D	0.97	C15C—H15I	0.96
C2B—C5B	1.5252 (18)	C16C—H16G	0.96

C2B—C3B	1.5329 (17)	C16C—H16H	0.96
C2B—H2B	0.98	C16C—H16I	0.96
C3B—C7B	1.5128 (17)	C17C—C18C	1.5365 (17)
C3B—C4B	1.5376 (18)	C17C—H17E	0.97
C3B—H3B	0.98	C17C—H17F	0.97
C4B—H4C	0.97	C18C—C22C	1.5267 (19)
C4B—H4D	0.97	C18C—C21C	1.5271 (18)
C5B—C15B	1.5175 (17)	C18C—C19C	1.5320 (17)
C5B—C16B	1.5208 (18)	C19C—C20C	1.5110 (17)
C6B—C7B	1.3559 (16)	C19C—H19E	0.97
C6B—C17B	1.4996 (17)	C19C—H19F	0.97
C7B—C20B	1.4588 (17)	C21C—H21G	0.96
C8B—C13B	1.3909 (18)	C21C—H21H	0.96
C8B—C9B	1.3938 (18)	C21C—H21I	0.96
C9B—C10B	1.3926 (19)	C22C—H22G	0.96
C9B—H9B	0.93	C22C—H22H	0.96
C10B—C11B	1.3950 (19)	C22C—H22I	0.96
O1A—S1A—O2A	120.18 (6)	C13B—C12B—C11B	120.90 (12)
O1A—S1A—N1A	106.92 (6)	C13B—C12B—H12B	119.6
O2A—S1A—N1A	105.63 (6)	C11B—C12B—H12B	119.6
O1A—S1A—C8A	107.95 (6)	C12B—C13B—C8B	119.66 (13)
O2A—S1A—C8A	107.94 (6)	C12B—C13B—H13B	120.2
N1A—S1A—C8A	107.64 (6)	C8B—C13B—H13B	120.2
C6A—O3A—C5A	117.82 (9)	C11B—C14B—H14D	109.5
C1A—N1A—C4A	110.35 (9)	C11B—C14B—H14E	109.5
C1A—N1A—S1A	120.18 (8)	H14D—C14B—H14E	109.5
C4A—N1A—S1A	117.47 (8)	C11B—C14B—H14F	109.5
N1A—C1A—C2A	101.06 (9)	H14D—C14B—H14F	109.5
N1A—C1A—H1A	111.6	H14E—C14B—H14F	109.5
C2A—C1A—H1A	111.6	C5B—C15B—H15D	109.5
N1A—C1A—H1B	111.6	C5B—C15B—H15E	109.5
C2A—C1A—H1B	111.6	H15D—C15B—H15E	109.5
H1A—C1A—H1B	109.4	C5B—C15B—H15F	109.5
C1A—C2A—C5A	114.93 (10)	H15D—C15B—H15F	109.5
C1A—C2A—C3A	103.59 (10)	H15E—C15B—H15F	109.5
C5A—C2A—C3A	113.38 (10)	C5B—C16B—H16D	109.5
C1A—C2A—H2A	108.2	C5B—C16B—H16E	109.5
C5A—C2A—H2A	108.2	H16D—C16B—H16E	109.5
C3A—C2A—H2A	108.2	C5B—C16B—H16F	109.5
C7A—C3A—C2A	110.51 (10)	H16D—C16B—H16F	109.5
C7A—C3A—C4A	112.84 (10)	H16E—C16B—H16F	109.5
C2A—C3A—C4A	104.08 (9)	C6B—C17B—C18B	112.09 (10)
C7A—C3A—H3A	109.8	C6B—C17B—H17C	109.2
C2A—C3A—H3A	109.8	C18B—C17B—H17C	109.2
C4A—C3A—H3A	109.8	C6B—C17B—H17D	109.2
N1A—C4A—C3A	104.35 (9)	C18B—C17B—H17D	109.2
N1A—C4A—H4A	110.9	H17C—C17B—H17D	107.9
C3A—C4A—H4A	110.9	C21B—C18B—C22B	108.94 (10)
N1A—C4A—H4B	110.9	C21B—C18B—C19B	110.35 (10)

C3A—C4A—H4B	110.9	C22B—C18B—C19B	111.29 (10)
H4A—C4A—H4B	108.9	C21B—C18B—C17B	109.25 (10)
O3A—C5A—C15A	103.84 (9)	C22B—C18B—C17B	109.54 (10)
O3A—C5A—C16A	107.99 (10)	C19B—C18B—C17B	107.44 (10)
C15A—C5A—C16A	111.47 (11)	C20B—C19B—C18B	115.13 (10)
O3A—C5A—C2A	109.93 (10)	C20B—C19B—H19C	108.5
C15A—C5A—C2A	112.56 (10)	C18B—C19B—H19C	108.5
C16A—C5A—C2A	110.73 (10)	C20B—C19B—H19D	108.5
O3A—C6A—C7A	124.19 (11)	C18B—C19B—H19D	108.5
O3A—C6A—C17A	111.25 (10)	H19C—C19B—H19D	107.5
C7A—C6A—C17A	124.56 (11)	O4B—C20B—C7B	121.17 (12)
C6A—C7A—C20A	118.57 (11)	O4B—C20B—C19B	120.14 (11)
C6A—C7A—C3A	122.42 (11)	C7B—C20B—C19B	118.69 (10)
C20A—C7A—C3A	118.98 (10)	C18B—C21B—H21D	109.5
C9A—C8A—C13A	120.71 (12)	C18B—C21B—H21E	109.5
C9A—C8A—S1A	119.88 (10)	H21D—C21B—H21E	109.5
C13A—C8A—S1A	119.40 (10)	C18B—C21B—H21F	109.5
C8A—C9A—C10A	119.26 (12)	H21D—C21B—H21F	109.5
C8A—C9A—H9A	120.4	H21E—C21B—H21F	109.5
C10A—C9A—H9A	120.4	C18B—C22B—H22D	109.5
C9A—C10A—C11A	120.96 (12)	C18B—C22B—H22E	109.5
C9A—C10A—H10A	119.5	H22D—C22B—H22E	109.5
C11A—C10A—H10A	119.5	C18B—C22B—H22F	109.5
C12A—C11A—C10A	118.61 (12)	H22D—C22B—H22F	109.5
C12A—C11A—C14A	121.03 (12)	H22E—C22B—H22F	109.5
C10A—C11A—C14A	120.36 (12)	O2C—S1C—O1C	120.06 (6)
C11A—C12A—C13A	121.44 (12)	O2C—S1C—N1C	106.19 (6)
C11A—C12A—H12A	119.3	O1C—S1C—N1C	106.49 (6)
C13A—C12A—H12A	119.3	O2C—S1C—C8C	107.60 (6)
C12A—C13A—C8A	119.00 (12)	O1C—S1C—C8C	107.15 (6)
C12A—C13A—H13A	120.5	N1C—S1C—C8C	109.01 (6)
C8A—C13A—H13A	120.5	C6C—O3C—C5C	117.58 (9)
C11A—C14A—H14A	109.5	C1C—N1C—C4C	111.13 (10)
C11A—C14A—H14B	109.5	C1C—N1C—S1C	118.85 (8)
H14A—C14A—H14B	109.5	C4C—N1C—S1C	119.80 (8)
C11A—C14A—H14C	109.5	N1C—C1C—C2C	103.70 (10)
H14A—C14A—H14C	109.5	N1C—C1C—H1E	111.0
H14B—C14A—H14C	109.5	C2C—C1C—H1E	111.0
C5A—C15A—H15A	109.5	N1C—C1C—H1F	111.0
C5A—C15A—H15B	109.5	C2C—C1C—H1F	111.0
H15A—C15A—H15B	109.5	H1E—C1C—H1F	109.0
C5A—C15A—H15C	109.5	C5C—C2C—C1C	112.87 (10)
H15A—C15A—H15C	109.5	C5C—C2C—C3C	112.68 (10)
H15B—C15A—H15C	109.5	C1C—C2C—C3C	104.27 (10)
C5A—C16A—H16A	109.5	C5C—C2C—H2C	109.0
C5A—C16A—H16B	109.5	C1C—C2C—H2C	109.0
H16A—C16A—H16B	109.5	C3C—C2C—H2C	109.0
C5A—C16A—H16C	109.5	C7C—C3C—C4C	112.76 (10)
H16A—C16A—H16C	109.5	C7C—C3C—C2C	110.05 (10)

H16B—C16A—H16C	109.5	C4C—C3C—C2C	102.80 (10)
C6A—C17A—C18A	113.35 (10)	C7C—C3C—H3C	110.3
C6A—C17A—H17A	108.9	C4C—C3C—H3C	110.3
C18A—C17A—H17A	108.9	C2C—C3C—H3C	110.3
C6A—C17A—H17B	108.9	N1C—C4C—C3C	104.62 (9)
C18A—C17A—H17B	108.9	N1C—C4C—H4E	110.8
H17A—C17A—H17B	107.7	C3C—C4C—H4E	110.8
C22A—C18A—C19A	109.92 (10)	N1C—C4C—H4F	110.8
C22A—C18A—C17A	109.41 (10)	C3C—C4C—H4F	110.8
C19A—C18A—C17A	107.65 (10)	H4E—C4C—H4F	108.9
C22A—C18A—C21A	109.09 (11)	O3C—C5C—C15C	104.35 (10)
C19A—C18A—C21A	110.41 (11)	O3C—C5C—C16C	107.86 (10)
C17A—C18A—C21A	110.33 (10)	C15C—C5C—C16C	111.01 (11)
C20A—C19A—C18A	114.55 (10)	O3C—C5C—C2C	109.23 (10)
C20A—C19A—H19A	108.6	C15C—C5C—C2C	112.52 (10)
C18A—C19A—H19A	108.6	C16C—C5C—C2C	111.51 (10)
C20A—C19A—H19B	108.6	O3C—C6C—C7C	123.96 (11)
C18A—C19A—H19B	108.6	O3C—C6C—C17C	111.81 (10)
H19A—C19A—H19B	107.6	C7C—C6C—C17C	124.22 (11)
O4A—C20A—C7A	121.31 (11)	C6C—C7C—C20C	118.82 (11)
O4A—C20A—C19A	120.05 (11)	C6C—C7C—C3C	122.50 (11)
C7A—C20A—C19A	118.58 (10)	C20C—C7C—C3C	118.63 (10)
C18A—C21A—H21A	109.5	C9C—C8C—C13C	120.54 (12)
C18A—C21A—H21B	109.5	C9C—C8C—S1C	120.07 (10)
H21A—C21A—H21B	109.5	C13C—C8C—S1C	119.39 (10)
C18A—C21A—H21C	109.5	C8C—C9C—C10C	119.30 (12)
H21A—C21A—H21C	109.5	C8C—C9C—H9C	120.3
H21B—C21A—H21C	109.5	C10C—C9C—H9C	120.3
C18A—C22A—H22A	109.5	C9C—C10C—C11C	121.13 (12)
C18A—C22A—H22B	109.5	C9C—C10C—H10C	119.4
H22A—C22A—H22B	109.5	C11C—C10C—H10C	119.4
C18A—C22A—H22C	109.5	C12C—C11C—C10C	118.60 (12)
H22A—C22A—H22C	109.5	C12C—C11C—C14C	120.87 (12)
H22B—C22A—H22C	109.5	C10C—C11C—C14C	120.52 (13)
O2B—S1B—O1B	120.15 (6)	C13C—C12C—C11C	121.00 (12)
O2B—S1B—N1B	106.45 (6)	C13C—C12C—H12C	119.5
O1B—S1B—N1B	106.65 (6)	C11C—C12C—H12C	119.5
O2B—S1B—C8B	108.33 (6)	C12C—C13C—C8C	119.40 (12)
O1B—S1B—C8B	107.35 (6)	C12C—C13C—H13C	120.3
N1B—S1B—C8B	107.29 (6)	C8C—C13C—H13C	120.3
C6B—O3B—C5B	116.93 (9)	C11C—C14C—H14G	109.5
C1B—N1B—C4B	111.34 (10)	C11C—C14C—H14H	109.5
C1B—N1B—S1B	118.83 (8)	H14G—C14C—H14H	109.5
C4B—N1B—S1B	119.41 (9)	C11C—C14C—H14I	109.5
N1B—C1B—C2B	103.30 (10)	H14G—C14C—H14I	109.5
N1B—C1B—H1C	111.1	H14H—C14C—H14I	109.5
C2B—C1B—H1C	111.1	C5C—C15C—H15G	109.5
N1B—C1B—H1D	111.1	C5C—C15C—H15H	109.5
C2B—C1B—H1D	111.1	H15G—C15C—H15H	109.5

H1C—C1B—H1D	109.1	C5C—C15C—H15I	109.5
C5B—C2B—C3B	112.70 (10)	H15G—C15C—H15I	109.5
C5B—C2B—C1B	112.84 (10)	H15H—C15C—H15I	109.5
C3B—C2B—C1B	104.55 (10)	C5C—C16C—H16G	109.5
C5B—C2B—H2B	108.9	C5C—C16C—H16H	109.5
C3B—C2B—H2B	108.9	H16G—C16C—H16H	109.5
C1B—C2B—H2B	108.9	C5C—C16C—H16I	109.5
C7B—C3B—C2B	110.04 (10)	H16G—C16C—H16I	109.5
C7B—C3B—C4B	113.36 (11)	H16H—C16C—H16I	109.5
C2B—C3B—C4B	102.89 (10)	C6C—C17C—C18C	112.49 (10)
C7B—C3B—H3B	110.1	C6C—C17C—H17E	109.1
C2B—C3B—H3B	110.1	C18C—C17C—H17E	109.1
C4B—C3B—H3B	110.1	C6C—C17C—H17F	109.1
N1B—C4B—C3B	104.67 (10)	C18C—C17C—H17F	109.1
N1B—C4B—H4C	110.8	H17E—C17C—H17F	107.8
C3B—C4B—H4C	110.8	C22C—C18C—C21C	109.50 (11)
N1B—C4B—H4D	110.8	C22C—C18C—C19C	110.95 (10)
C3B—C4B—H4D	110.8	C21C—C18C—C19C	108.92 (11)
H4C—C4B—H4D	108.9	C22C—C18C—C17C	109.72 (11)
O3B—C5B—C15B	104.31 (10)	C21C—C18C—C17C	109.80 (10)
O3B—C5B—C16B	107.68 (10)	C19C—C18C—C17C	107.92 (10)
C15B—C5B—C16B	111.02 (11)	C20C—C19C—C18C	115.16 (10)
O3B—C5B—C2B	109.24 (10)	C20C—C19C—H19E	108.5
C15B—C5B—C2B	112.69 (11)	C18C—C19C—H19E	108.5
C16B—C5B—C2B	111.52 (10)	C20C—C19C—H19F	108.5
O3B—C6B—C7B	123.96 (11)	C18C—C19C—H19F	108.5
O3B—C6B—C17B	111.91 (10)	H19E—C19C—H19F	107.5
C7B—C6B—C17B	124.13 (11)	O4C—C20C—C7C	120.99 (11)
C6B—C7B—C20B	118.76 (11)	O4C—C20C—C19C	120.38 (11)
C6B—C7B—C3B	122.51 (11)	C7C—C20C—C19C	118.63 (10)
C20B—C7B—C3B	118.60 (10)	C18C—C21C—H21G	109.5
C13B—C8B—C9B	120.30 (12)	C18C—C21C—H21H	109.5
C13B—C8B—S1B	119.57 (10)	H21G—C21C—H21H	109.5
C9B—C8B—S1B	120.11 (10)	C18C—C21C—H21I	109.5
C10B—C9B—C8B	119.34 (12)	H21G—C21C—H21I	109.5
C10B—C9B—H9B	120.3	H21H—C21C—H21I	109.5
C8B—C9B—H9B	120.3	C18C—C22C—H22G	109.5
C9B—C10B—C11B	120.95 (13)	C18C—C22C—H22H	109.5
C9B—C10B—H10B	119.5	H22G—C22C—H22H	109.5
C11B—C10B—H10B	119.5	C18C—C22C—H22I	109.5
C12B—C11B—C10B	118.83 (12)	H22G—C22C—H22I	109.5
C12B—C11B—C14B	120.55 (13)	H22H—C22C—H22I	109.5
C10B—C11B—C14B	120.61 (13)		
O1A—S1A—N1A—C1A	−45.96 (11)	C4B—C3B—C7B—C6B	122.83 (13)
O2A—S1A—N1A—C1A	−175.06 (9)	C2B—C3B—C7B—C20B	−176.04 (10)
C8A—S1A—N1A—C1A	69.81 (10)	C4B—C3B—C7B—C20B	−61.45 (14)
O1A—S1A—N1A—C4A	174.96 (9)	O2B—S1B—C8B—C13B	161.51 (10)
O2A—S1A—N1A—C4A	45.86 (10)	O1B—S1B—C8B—C13B	30.38 (12)
C8A—S1A—N1A—C4A	−69.27 (10)	N1B—S1B—C8B—C13B	−83.93 (11)

C4A—N1A—C1A—C2A	−34.00 (12)	O2B—S1B—C8B—C9B	−20.19 (12)
S1A—N1A—C1A—C2A	−175.70 (8)	O1B—S1B—C8B—C9B	−151.33 (11)
N1A—C1A—C2A—C5A	164.73 (10)	N1B—S1B—C8B—C9B	94.36 (11)
N1A—C1A—C2A—C3A	40.49 (11)	C13B—C8B—C9B—C10B	0.33 (19)
C1A—C2A—C3A—C7A	88.38 (11)	S1B—C8B—C9B—C10B	−177.95 (10)
C5A—C2A—C3A—C7A	−36.86 (14)	C8B—C9B—C10B—C11B	0.9 (2)
C1A—C2A—C3A—C4A	−33.03 (12)	C9B—C10B—C11B—C12B	−0.87 (19)
C5A—C2A—C3A—C4A	−158.27 (10)	C9B—C10B—C11B—C14B	178.33 (12)
C1A—N1A—C4A—C3A	13.58 (13)	C10B—C11B—C12B—C13B	−0.30 (19)
S1A—N1A—C4A—C3A	156.44 (8)	C14B—C11B—C12B—C13B	−179.50 (12)
C7A—C3A—C4A—N1A	−107.31 (11)	C11B—C12B—C13B—C8B	1.5 (2)
C2A—C3A—C4A—N1A	12.53 (12)	C9B—C8B—C13B—C12B	−1.48 (19)
C6A—O3A—C5A—C15A	−164.07 (10)	S1B—C8B—C13B—C12B	176.82 (10)
C6A—O3A—C5A—C16A	77.48 (13)	O3B—C6B—C17B—C18B	146.48 (10)
C6A—O3A—C5A—C2A	−43.43 (14)	C7B—C6B—C17B—C18B	−33.42 (16)
C1A—C2A—C5A—O3A	−65.07 (13)	C6B—C17B—C18B—C21B	171.38 (10)
C3A—C2A—C5A—O3A	53.83 (13)	C6B—C17B—C18B—C22B	−69.36 (13)
C1A—C2A—C5A—C15A	50.16 (14)	C6B—C17B—C18B—C19B	51.67 (13)
C3A—C2A—C5A—C15A	169.05 (10)	C21B—C18B—C19B—C20B	−169.58 (11)
C1A—C2A—C5A—C16A	175.69 (11)	C22B—C18B—C19B—C20B	69.35 (14)
C3A—C2A—C5A—C16A	−65.41 (13)	C17B—C18B—C19B—C20B	−50.57 (14)
C5A—O3A—C6A—C7A	16.51 (17)	C6B—C7B—C20B—O4B	174.67 (12)
C5A—O3A—C6A—C17A	−163.36 (10)	C3B—C7B—C20B—O4B	−1.21 (18)
O3A—C6A—C7A—C20A	−176.47 (11)	C6B—C7B—C20B—C19B	−5.13 (17)
C17A—C6A—C7A—C20A	3.39 (19)	C3B—C7B—C20B—C19B	178.99 (11)
O3A—C6A—C7A—C3A	1.69 (19)	C18B—C19B—C20B—O4B	−151.47 (12)
C17A—C6A—C7A—C3A	−178.45 (11)	C18B—C19B—C20B—C7B	28.34 (16)
C2A—C3A—C7A—C6A	9.35 (16)	O2C—S1C—N1C—C1C	173.66 (9)
C4A—C3A—C7A—C6A	125.42 (12)	O1C—S1C—N1C—C1C	44.61 (11)
C2A—C3A—C7A—C20A	−172.49 (10)	C8C—S1C—N1C—C1C	−70.68 (10)
C4A—C3A—C7A—C20A	−56.42 (14)	O2C—S1C—N1C—C4C	−44.19 (10)
O1A—S1A—C8A—C9A	−144.95 (10)	O1C—S1C—N1C—C4C	−173.23 (9)
O2A—S1A—C8A—C9A	−13.62 (12)	C8C—S1C—N1C—C4C	71.48 (10)
N1A—S1A—C8A—C9A	99.96 (11)	C4C—N1C—C1C—C2C	13.39 (13)
O1A—S1A—C8A—C13A	35.54 (12)	S1C—N1C—C1C—C2C	158.58 (8)
O2A—S1A—C8A—C13A	166.87 (10)	N1C—C1C—C2C—C5C	−153.75 (10)
N1A—S1A—C8A—C13A	−79.54 (11)	N1C—C1C—C2C—C3C	−31.13 (12)
C13A—C8A—C9A—C10A	−0.31 (19)	C5C—C2C—C3C—C7C	39.41 (13)
S1A—C8A—C9A—C10A	−179.81 (9)	C1C—C2C—C3C—C7C	−83.33 (11)
C8A—C9A—C10A—C11A	1.44 (19)	C5C—C2C—C3C—C4C	159.76 (10)
C9A—C10A—C11A—C12A	−1.30 (19)	C1C—C2C—C3C—C4C	37.02 (12)
C9A—C10A—C11A—C14A	178.36 (12)	C1C—N1C—C4C—C3C	9.68 (13)
C10A—C11A—C12A—C13A	0.03 (19)	S1C—N1C—C4C—C3C	−135.15 (9)
C14A—C11A—C12A—C13A	−179.63 (12)	C7C—C3C—C4C—N1C	89.95 (12)
C11A—C12A—C13A—C8A	1.07 (19)	C2C—C3C—C4C—N1C	−28.52 (12)
C9A—C8A—C13A—C12A	−0.92 (19)	C6C—O3C—C5C—C15C	164.37 (10)
S1A—C8A—C13A—C12A	178.58 (10)	C6C—O3C—C5C—C16C	−77.51 (13)
O3A—C6A—C17A—C18A	−157.46 (10)	C6C—O3C—C5C—C2C	43.85 (13)
C7A—C6A—C17A—C18A	22.67 (18)	C1C—C2C—C5C—O3C	61.06 (13)

C6A—C17A—C18A—C22A	−167.78 (11)	C3C—C2C—C5C—O3C	−56.72 (13)
C6A—C17A—C18A—C19A	−48.36 (14)	C1C—C2C—C5C—C15C	−54.34 (14)
C6A—C17A—C18A—C21A	72.19 (13)	C3C—C2C—C5C—C15C	−172.12 (10)
C22A—C18A—C19A—C20A	171.53 (11)	C1C—C2C—C5C—C16C	−179.82 (11)
C17A—C18A—C19A—C20A	52.44 (14)	C3C—C2C—C5C—C16C	62.40 (14)
C21A—C18A—C19A—C20A	−68.06 (14)	C5C—O3C—C6C—C7C	−14.29 (17)
C6A—C7A—C20A—O4A	177.36 (12)	C5C—O3C—C6C—C17C	166.96 (10)
C3A—C7A—C20A—O4A	−0.87 (18)	O3C—C6C—C7C—C20C	172.98 (11)
C6A—C7A—C20A—C19A	0.04 (17)	C17C—C6C—C7C—C20C	−8.43 (18)
C3A—C7A—C20A—C19A	−178.19 (11)	O3C—C6C—C7C—C3C	−4.26 (19)
C18A—C19A—C20A—O4A	153.01 (12)	C17C—C6C—C7C—C3C	174.34 (11)
C18A—C19A—C20A—C7A	−29.63 (16)	C4C—C3C—C7C—C6C	−123.50 (13)
O2B—S1B—N1B—C1B	−173.78 (9)	C2C—C3C—C7C—C6C	−9.36 (16)
O1B—S1B—N1B—C1B	−44.36 (11)	C4C—C3C—C7C—C20C	59.26 (14)
C8B—S1B—N1B—C1B	70.41 (10)	C2C—C3C—C7C—C20C	173.40 (10)
O2B—S1B—N1B—C4B	44.31 (11)	O2C—S1C—C8C—C9C	15.46 (12)
O1B—S1B—N1B—C4B	173.73 (9)	O1C—S1C—C8C—C9C	145.84 (11)
C8B—S1B—N1B—C4B	−71.49 (10)	N1C—S1C—C8C—C9C	−99.30 (11)
C4B—N1B—C1B—C2B	−13.96 (13)	O2C—S1C—C8C—C13C	−163.64 (10)
S1B—N1B—C1B—C2B	−158.72 (9)	O1C—S1C—C8C—C13C	−33.26 (12)
N1B—C1B—C2B—C5B	154.09 (10)	N1C—S1C—C8C—C13C	81.61 (11)
N1B—C1B—C2B—C3B	31.27 (12)	C13C—C8C—C9C—C10C	0.6 (2)
C5B—C2B—C3B—C7B	−38.52 (14)	S1C—C8C—C9C—C10C	−178.52 (10)
C1B—C2B—C3B—C7B	84.39 (12)	C8C—C9C—C10C—C11C	−1.2 (2)
C5B—C2B—C3B—C4B	−159.61 (10)	C9C—C10C—C11C—C12C	0.5 (2)
C1B—C2B—C3B—C4B	−36.70 (12)	C9C—C10C—C11C—C14C	179.85 (12)
C1B—N1B—C4B—C3B	−8.77 (14)	C10C—C11C—C12C—C13C	0.9 (2)
S1B—N1B—C4B—C3B	135.76 (9)	C14C—C11C—C12C—C13C	−178.45 (12)
C7B—C3B—C4B—N1B	−91.02 (12)	C11C—C12C—C13C—C8C	−1.6 (2)
C2B—C3B—C4B—N1B	27.78 (12)	C9C—C8C—C13C—C12C	0.80 (19)
C6B—O3B—C5B—C15B	−166.34 (10)	S1C—C8C—C13C—C12C	179.89 (10)
C6B—O3B—C5B—C16B	75.64 (13)	O3C—C6C—C17C—C18C	−149.76 (10)
C6B—O3B—C5B—C2B	−45.63 (13)	C7C—C6C—C17C—C18C	31.49 (17)
C3B—C2B—C5B—O3B	57.36 (13)	C6C—C17C—C18C—C22C	71.25 (13)
C1B—C2B—C5B—O3B	−60.78 (13)	C6C—C17C—C18C—C21C	−168.35 (11)
C3B—C2B—C5B—C15B	172.81 (10)	C6C—C17C—C18C—C19C	−49.75 (14)
C1B—C2B—C5B—C15B	54.66 (14)	C22C—C18C—C19C—C20C	−69.78 (14)
C3B—C2B—C5B—C16B	−61.54 (14)	C21C—C18C—C19C—C20C	169.61 (11)
C1B—C2B—C5B—C16B	−179.68 (11)	C17C—C18C—C19C—C20C	50.45 (14)
C5B—O3B—C6B—C7B	15.91 (17)	C6C—C7C—C20C—O4C	−173.46 (12)
C5B—O3B—C6B—C17B	−164.00 (10)	C3C—C7C—C20C—O4C	3.88 (18)
O3B—C6B—C7B—C20B	−171.63 (11)	C6C—C7C—C20C—C19C	7.21 (17)
C17B—C6B—C7B—C20B	8.27 (18)	C3C—C7C—C20C—C19C	−175.45 (10)
O3B—C6B—C7B—C3B	4.08 (19)	C18C—C19C—C20C—O4C	150.50 (12)
C17B—C6B—C7B—C3B	−176.02 (11)	C18C—C19C—C20C—C7C	−30.17 (16)
C2B—C3B—C7B—C6B	8.24 (16)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2A—H2A···O1C	0.98	2.51	3.4447 (18)	160
C2B—H2B···O1B^{i}	0.98	2.52	3.4167 (18)	151
C2C—H2C···O1A	0.98	2.51	3.4739 (18)	167
C4A—H4A···O4A	0.97	2.48	2.9605 (17)	111
C4B—H4C···O4B	0.97	2.48	3.0370 (18)	116
C4C—H4F···O4C	0.97	2.43	3.0069 (17)	118
C12A—H12A···O2C^{ii}	0.93	2.51	3.2130 (16)	133
C12B—H12B···O2A^{iii}	0.93	2.59	3.3762 (18)	143
C14C—H14I···O2C^{iv}	0.96	2.56	3.362 (2)	142
C17A—H17B···O4C^{ii}	0.97	2.51	3.3480 (18)	145
C17B—H17C···O4A^{iii}	0.97	2.38	3.2776 (17)	154
C21C—H21I···O4B^{v}	0.96	2.47	3.3058 (17)	146
C22A—H22B···O4C^{ii}	0.96	2.55	3.4023 (16)	147

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

Fig. 1

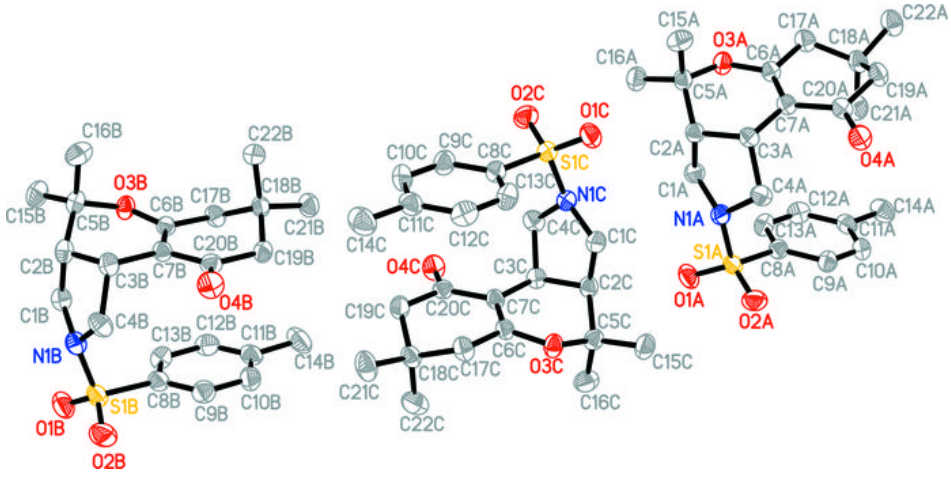

C16B
C22B
O3B
C6B
C17B
C18B
C15B
C5B
C21B
C20B
C2B
C3B
C7B
C19B
O4B
C1B
C4B
C13B
C12B
C11B
C14B
N1B
S1B
C8B
C9B
C10B
O1B
O2B
C10C
C9C
C8C
S1C
O2C
O1C
C13C
N1C
C14C
C11C
C12C
C4C
C1C
O4C
C3C
C2C
C19C
C20C
C7C
C5C
C6C
O3C
C15C
C21C
C18C
C17C
C16C
C22C
C15A
O3A
C17A
C18A
C22A
C16A
C6A
C5A
C20A
C19A
C21A
C7A
C2A
C3A
O4A
C1A
C4A
C12A
C14A
N1A
C13A
C11A
S1A
C8A
C9A
C10A
O1A
O2A

Fig. 2

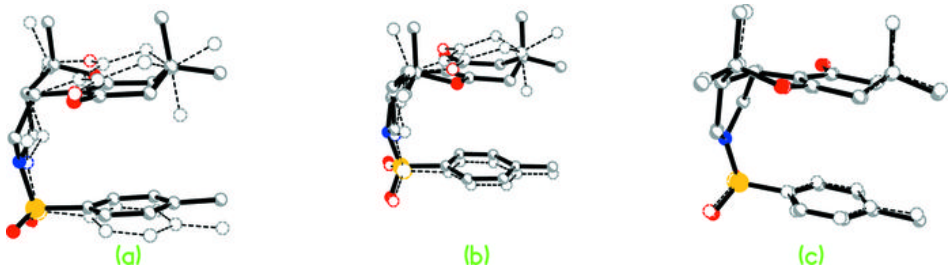
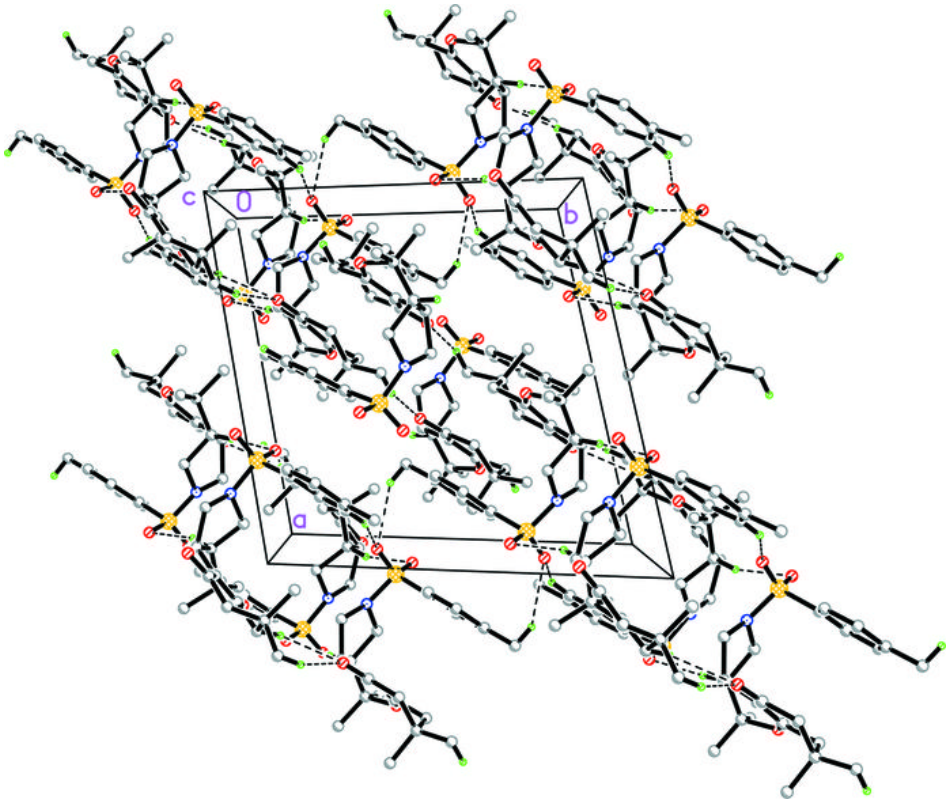


Fig. 3



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