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trans-1-Ethyl-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

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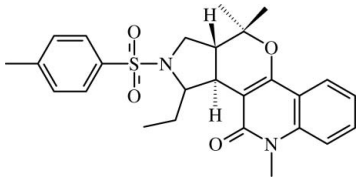
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.004 Å; R factor = 0.067; wR factor = 0.166; data-to-parameter ratio = 22.7.

The asymmetric unit of the title compound, $C_{26}H_{30}N_2O_4S$, consists of two independent molecules, *A* and *B*, with similar conformations. In both molecules, the pyrrolidine and dihydropyran rings adopt envelope conformations, and are *trans*-fused; the tosyl group is attached to the pyrrolidine ring in a biaxial position and the sulfonyl group has distorted tetrahedral geometry. The *A* molecules are linked into a chain along the *b* axis by C—H···O hydrogen bonds, and the inversion-related molecules of adjacent chains are cross-linked into a two-dimensional network parallel to the *bc* plane *via* C—H···π interactions involving the pyridinone ring, and π–π interactions involving the benzene ring of the quinolinone ring system. A similar two-dimensional network is also formed by the *B* molecules. The centroid–centroid distances for the π–π interactions in the *A* and B molecules are 3.5477 (13) and 3.5743 (15) Å, respectively. The two-dimensional networks formed by the *A* and *B* molecules are arranged alternately along the *a* axis, and are linked *via* C—H···π interactions involving the sulfonyl-bound benzene ring of molecule *B*.

Related literature

For the *cis*-isomer, see: Chinnakali *et al.* (2007). For ring puckering parameters, see: Cremer & Pople (1975). For asymmetry parameters, see: Duax *et al.* (1976).



Experimental

Crystal data

$C_{26}H_{30}N_2O_4S$
M_r = 466.58
Monoclinic, $P2_1/c$
a = 24.7027 (7) Å
b = 10.2685 (3) Å
c = 19.6195 (5) Å
β = 109.554 (1)°
V = 4689.7 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.17 mm^{-1}
T = 100.0 (1) K
0.29 × 0.20 × 0.10 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.951, T_{max} = 0.983
45928 measured reflections
13623 independent reflections
9445 reflections with $I > 2\sigma(I)$
R_{int} = 0.055

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.166
S = 1.02
13623 reflections
599 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

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

*Cg*1, *Cg*2, *Cg*4 and *Cg*5 are the centroids of the N2*A*/C22*A*/C17*A*/C6*A*/C7*A*/C23*A*, C8*A*–C13*A*, N2*B*/C22*B*/C17*B*/C6*B*/C7*B*/C23*B* and C8*B*–C13*B* rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C25*A*—H25*A*···O4*A*	0.97	2.27	2.915 (3)	123
C25*A*—H25*B*···O2*A*	0.97	2.53	3.182 (3)	125
C25*B*—H25*C*···O4*B*	0.97	2.29	2.916 (4)	121
C25*B*—H25*D*···O2*B*	0.97	2.52	3.170 (4)	124
C10*A*—H10*A*···O4*A*^{i}	0.93	2.41	3.279 (3)	155
C24*A*—H24*A*···O2*A*^{i}	0.96	2.58	3.466 (3)	153
C10*B*—H10*B*···O4*B*^{ii}	0.93	2.36	3.273 (4)	167
C24*B*—H24*E*···O2*B*^{ii}	0.96	2.49	3.406 (4)	159
C16*A*—H16*C*···*Cg*1^{iii}	0.96	2.81	3.416 (2)	122
C20*A*—H20*A*···*Cg*2^{iv}	0.93	2.87	3.631 (3)	140
C16*B*—H16*D*···*Cg*4^{v}	0.96	2.90	3.612 (3)	131
C20*B*—H20*B*···*Cg*5^{vi}	0.93	2.82	3.589 (3)	141
C12*A*—H12*A*···*Cg*5^{vii}	0.93	2.87	3.782 (3)	166

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

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).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2215).

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supplementary materials

Acta Cryst. (2007). E**63**, o4650-o4651 [**doi:10.1107/S1600536807054906**]

trans-1-Ethyl-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

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

Comment

Previously, we have reported the crystal structure of *cis*-1-ethyl-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 (Chinnakali *et al.*, 2007). Now we report the crystal structure of the title compound, the *trans*-isomer.

The asymmetric unit of the title compound consists of two independent molecules, *A* and *B*, with quite 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 0.086 Å. The pyrrolidine ring in both molecules is *trans*-fused to the dihydropyran ring.

The pyrrolidine ring in each molecule *A* and *B* adopts an envelope conformation, with the local mirror plane passing through C2 and the mid-point of the bond N1—C4. The relevant asymmetry parameters (Duax *et al.*, 1976) are ΔC_s[C2] = 5.8 (2)° for molecule *A* and 6.0 (2)° for molecule *B*; the puckering parameters Q and φ (Cremer & Pople, 1975) are 0.438 (2) Å and 78.9 (3)° for molecule *A*, and 0.429 (3) Å and 79.3 (3)° for molecule *B*. In the *cis*-isomer, the pyrrolidine ring adopts a twist conformation. In both molecules, the tosyl group is attached to the pyrrolidine ring in a biaxial position. The sum of the bond angles around atom N1 of the molecules *A* (345.6°) and *B* (348.0°) indicates sp^3 hybridization.

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 5.2 (2)° for molecule *A* and 1.1 (2)° for molecule *B*; the puckering parameters Q, θ and φ are 0.493 (2) Å, 128.6 (2)° and 294.1 (3)° for molecule *A*, and 0.486 (3) Å, 128.0 (2)° and 299.1 (4)° for molecule *B*. In the *cis*-isomer, the dihydropyran ring is in a half-chair conformation. In both molecules, the sulfonyl group has distorted tetrahedral geometry [O2A—S1A—O1A = 120.04 (11)° and O2B—S1B—O1B = 120.47 (12)°]; the quinolinone ring system is planar, with an r.m.s. deviation of 0.026 Å in molecule A and 0.014 Å in molecule B.

A superposition of the non-H atoms in the quinolinone ring systems of molecule *A* or *B* and *cis*-isomer (Chinnakali *et al.*, 2007) (Fig. 2) shows that the overall conformations of the *cis* and *trans* isomers are different. In the *cis*-isomer, the molecule is in a folded conformation, with the sulfonyl-bound phenyl ring lying over the pyridinone ring. But in the *trans*-isomer, though the tosyl group is slightly bent towards the fused ring system, it is not lying over the pyridinone ring. The *trans*-fusion results in an extended ring system.

The *A* molecules are linked into a chain along the *b* axis by C10A—H10A···O4A^{i} and C24A—H24A···O2A^{i} hydrogen bonds (symmetry code as in Table 1). Inversion-related molecules of the adjacent *A* chains are cross-linked into a two-dimensional network parallel to the *bc* plane *via* C16A—H16C···π interactions involving the N2A/C22A/C17A/C6A/C7A/C23A ring (centroid *Cg*1) of the molecules at (1 − *x*, 1 − *y*, 1 − *z*), C20A—H20A···π interactions involving the C8A—C13A ring (centroid *Cg*2) of the molecules at (1 − *x*, −*y*, 1 − *z*), and π-π interactions involving the C17A—C22A rings (centroid *Cg*3) of the molecules at (*x*, *y*, *z*) and (1 − *x*,-*y*,1 − *z*) [centroid-centroid distance is 3.5477 (13) Å].

Similarly, the *B* molecules are linked into a chain along the *b* axis by C10B—H10B···O4B^{ii} and C24B—H24E···O2B^{ii} hydrogen bonds (symmetry code as in Table 1). Inversion-related molecules of the adjacent B chains are cross-linked into a two-dimensional network parallel to the *bc* plane *via* C16B—H16D···π interactions involving the N2B/C22B/C17B/C6B/C7B/C23B ring (centroid *Cg*4) of the molecules at (−*x*, 1 − *y*, 1 − *z*), C20B—H20B···π interactions involving the C8B—C13B ring (centroid *Cg*5) of the molecules at (−*x*, 2 − *y*, 1 − *z*), and π-π interactions involving the C17B—C22B ring (centroid *Cg*6) of the molecules at (*x*, *y*, *z*) and (−*x*,2 − *y*,1 − *z*) [centroid-centroid distance is 3.5743 (15) Å].

The two-dimensional networks formed by the *A* and *B* molecules are arranged alternately along the *a* axis, and are linked *via* C12A—H12A···π interactions involving the C8B—C13B ring (centroid *Cg*5).

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]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

H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93–0.98 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C_{methyl}). A rotating group model was used for the methyl groups attached to aromatic rings. The displacement ellipsoid of methyl carbon atom C14B is unusually elongated and some of the U^{ij} components have large values. Attempts to restrain the U^{ij} components of C14B failed to improve the values. Hence the restraints were removed.

Figures

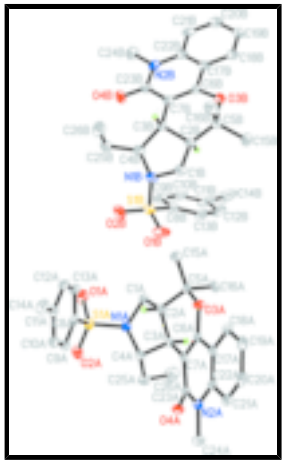

Fig. 1. The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 80% probability level. Hydrogen bonds are shown as dashed lines. All H atoms, except those at a ring junction, have been omitted for clarity.

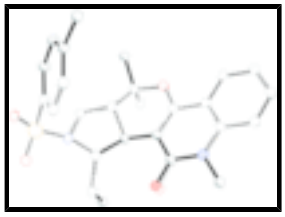

Fig. 2. Fit of molecule A (dashed lines) on molecule B (solid lines). H atoms have been omitted for clarity.

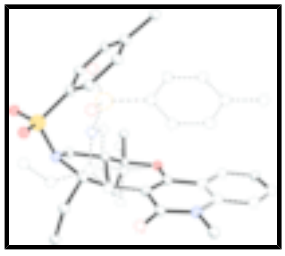

Fig. 3. Fit of molecule A (solid lines) in the title compound on a molecule of the *cis*-isomer (dashed lines). H atoms have been omitted for clarity.

trans-1-Ethyl-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

Crystal data

$C_{26}H_{30}N_2O_4S$	F_{000} = 1984
M_r = 466.58	D_x = 1.322 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 7777 reflections
a = 24.7027 (7) Å	θ = 2.3–29.5º
b = 10.2685 (3) Å	μ = 0.17 mm^{-1}
c = 19.6195 (5) Å	T = 100.0 (1) K
β = 109.554 (1)º	Plate, colourless
V = 4689.7 (2) Å^3	0.29 × 0.20 × 0.10 mm
Z = 8	

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer	13623 independent reflections
Radiation source: fine-focus sealed tube	9445 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.055
Detector resolution: 8.33 pixels mm^{-1}	θ_{max} = 30.1º
T = 100.0(1) K	θ_{min} = 0.9º
ω scans	h = −34→22
Absorption correction: multi-scan (SADABS; Bruker, 2005)	k = −14→11
T_{min} = 0.951, T_{max} = 0.983	l = −16→27
45928 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
$R[F^2 > 2\sigma(F^2)] = 0.067$	H-atom parameters constrained
$wR(F^2) = 0.166$	$w = 1/[\sigma^2(F_o^2) + (0.0598P)^2 + 5.1486P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} = 0.001$
13623 reflections	$\Delta\rho_{max} = 0.44$ e Å^{-3}
599 parameters	$\Delta\rho_{min} = -0.47$ 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 $F^2 > 2$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	0.31763 (3)	0.36357 (6)	0.17299 (3)	0.01999 (13)
O1A	0.26114 (8)	0.41782 (17)	0.15589 (9)	0.0269 (4)
O2A	0.34738 (8)	0.37166 (17)	0.12168 (9)	0.0283 (4)
O3A	0.42201 (7)	0.28125 (15)	0.48549 (8)	0.0180 (3)
O4A	0.54792 (7)	0.35142 (17)	0.35169 (9)	0.0230 (4)
N1A	0.35808 (8)	0.43454 (18)	0.24673 (10)	0.0170 (4)
N2A	0.57206 (8)	0.20597 (18)	0.44420 (10)	0.0166 (4)
C1A	0.33462 (10)	0.4457 (2)	0.30734 (12)	0.0175 (4)
H1A	0.2960	0.4108	0.2939	0.021*
H1B	0.3345	0.5354	0.3228	0.021*
C2A	0.37659 (9)	0.3639 (2)	0.36535 (11)	0.0143 (4)
H2A	0.3694	0.2729	0.3501	0.017*
C3A	0.43420 (9)	0.4014 (2)	0.35816 (11)	0.0143 (4)
H3A	0.4427	0.4916	0.3747	0.017*
C4A	0.42151 (9)	0.3987 (2)	0.27559 (12)	0.0176 (4)
H4A	0.4263	0.3095	0.2608	0.021*
C5A	0.37685 (9)	0.3709 (2)	0.44271 (12)	0.0150 (4)

C6A	0.46979 (9)	0.2629 (2)	0.46756 (12)	0.0153 (4)
C7A	0.47945 (9)	0.3147 (2)	0.40861 (12)	0.0143 (4)
C8A	0.31342 (10)	0.1962 (2)	0.19265 (12)	0.0171 (4)
C9A	0.35113 (10)	0.1081 (2)	0.17899 (13)	0.0215 (5)
H9A	0.3778	0.1358	0.1580	0.026*
C10A	0.34866 (10)	−0.0227 (2)	0.19714 (13)	0.0219 (5)
H10A	0.3739	−0.0819	0.1880	0.026*
C11A	0.30937 (10)	−0.0658 (2)	0.22845 (13)	0.0202 (5)
C12A	0.27156 (10)	0.0240 (2)	0.24137 (13)	0.0202 (5)
H12A	0.2448	−0.0037	0.2622	0.024*
C13A	0.27346 (10)	0.1543 (2)	0.22350 (13)	0.0211 (5)
H13A	0.2480	0.2134	0.2322	0.025*
C14A	0.30883 (11)	−0.2061 (2)	0.25107 (15)	0.0274 (5)
H14A	0.3135	−0.2620	0.2142	0.041*
H14B	0.2729	−0.2250	0.2578	0.041*
H14C	0.3397	−0.2207	0.2956	0.041*
C15A	0.32242 (10)	0.3164 (2)	0.45037 (13)	0.0202 (5)
H15A	0.3149	0.2320	0.4282	0.030*
H15B	0.2909	0.3736	0.4271	0.030*
H15C	0.3268	0.3091	0.5007	0.030*
C16A	0.39049 (11)	0.5049 (2)	0.47712 (13)	0.0224 (5)
H16A	0.3898	0.5014	0.5257	0.034*
H16B	0.3623	0.5663	0.4496	0.034*
H16C	0.4279	0.5315	0.4778	0.034*
C17A	0.51136 (9)	0.1791 (2)	0.51761 (12)	0.0156 (4)
C18A	0.50194 (10)	0.1239 (2)	0.57826 (12)	0.0187 (4)
H18A	0.4682	0.1423	0.5875	0.022*
C19A	0.54223 (11)	0.0429 (2)	0.62398 (13)	0.0218 (5)
H19A	0.5359	0.0070	0.6642	0.026*
C20A	0.59258 (10)	0.0149 (2)	0.60966 (13)	0.0216 (5)
H20A	0.6195	−0.0407	0.6404	0.026*
C21A	0.60328 (10)	0.0677 (2)	0.55114 (13)	0.0194 (5)
H21A	0.6373	0.0486	0.5428	0.023*
C22A	0.56250 (9)	0.1510 (2)	0.50379 (12)	0.0165 (4)
C23A	0.53431 (9)	0.2938 (2)	0.39858 (12)	0.0163 (4)
C24A	0.62589 (10)	0.1806 (3)	0.43081 (14)	0.0248 (5)
H24A	0.6329	0.0885	0.4326	0.037*
H24B	0.6569	0.2233	0.4671	0.037*
H24C	0.6232	0.2133	0.3839	0.037*
C25A	0.45550 (11)	0.4913 (3)	0.24427 (14)	0.0261 (5)
H25A	0.4921	0.4510	0.2489	0.031*
H25B	0.4347	0.5024	0.1931	0.031*
C26A	0.46692 (14)	0.6248 (3)	0.27936 (17)	0.0380 (7)
H26A	0.4884	0.6763	0.2565	0.057*
H26B	0.4885	0.6155	0.3299	0.057*
H26C	0.4310	0.6670	0.2740	0.057*
S1B	0.17892 (3)	0.62891 (6)	0.32745 (4)	0.02446 (14)
O1B	0.23600 (8)	0.57809 (18)	0.35872 (11)	0.0349 (5)
O2B	0.14798 (9)	0.6121 (2)	0.25207 (10)	0.0363 (5)

O3B	0.07962 (7)	0.72509 (16)	0.55757 (9)	0.0224 (4)
O4B	−0.04453 (8)	0.6673 (2)	0.31508 (10)	0.0323 (4)
N1B	0.14028 (9)	0.56320 (19)	0.37157 (11)	0.0211 (4)
N2B	−0.07210 (8)	0.79519 (19)	0.39207 (11)	0.0211 (4)
C1B	0.16564 (11)	0.5594 (2)	0.45133 (14)	0.0239 (5)
H1C	0.2040	0.5964	0.4679	0.029*
H1D	0.1672	0.4711	0.4695	0.029*
C2B	0.12392 (10)	0.6426 (2)	0.47433 (13)	0.0192 (5)
H2B	0.1302	0.7332	0.4630	0.023*
C3B	0.06602 (10)	0.6014 (2)	0.42108 (12)	0.0184 (4)
H3B	0.0583	0.5123	0.4332	0.022*
C4B	0.07693 (10)	0.5972 (2)	0.34795 (13)	0.0214 (5)
H4B	0.0713	0.6847	0.3267	0.026*
C5B	0.12589 (10)	0.6398 (2)	0.55229 (13)	0.0204 (5)
C6B	0.03148 (10)	0.7423 (2)	0.49971 (13)	0.0181 (4)
C7B	0.02111 (10)	0.6893 (2)	0.43303 (13)	0.0190 (5)
C8B	0.18260 (10)	0.7985 (2)	0.34440 (14)	0.0238 (5)
C9B	0.14173 (11)	0.8800 (3)	0.29762 (16)	0.0291 (6)
H9B	0.1139	0.8465	0.2567	0.035*
C10B	0.14328 (12)	1.0119 (3)	0.3131 (2)	0.0408 (8)
H10B	0.1163	1.0668	0.2819	0.049*
C11B	0.18375 (13)	1.0639 (3)	0.3735 (2)	0.0462 (9)
C12B	0.22467 (12)	0.9812 (3)	0.4189 (2)	0.0444 (8)
H12B	0.2526	1.0150	0.4596	0.053*
C13B	0.22450 (11)	0.8488 (3)	0.40430 (16)	0.0304 (6)
H13B	0.2524	0.7946	0.4346	0.037*
C14B	0.18209 (16)	1.2055 (3)	0.3921 (3)	0.0892 (18)
H14D	0.1448	1.2266	0.3943	0.134*
H14E	0.1896	1.2579	0.3557	0.134*
H14F	0.2108	1.2226	0.4382	0.134*
C15B	0.18005 (11)	0.7030 (3)	0.60244 (14)	0.0286 (6)
H15D	0.1850	0.7869	0.5837	0.043*
H15E	0.2126	0.6490	0.6057	0.043*
H15F	0.1769	0.7130	0.6496	0.043*
C16B	0.11612 (12)	0.5061 (3)	0.57967 (14)	0.0293 (6)
H16D	0.0816	0.4687	0.5468	0.044*
H16E	0.1125	0.5146	0.6267	0.044*
H16F	0.1481	0.4506	0.5828	0.044*
C17B	−0.00982 (10)	0.8270 (2)	0.51506 (13)	0.0199 (5)
C18B	0.00104 (11)	0.8865 (2)	0.58266 (14)	0.0222 (5)
H18B	0.0358	0.8714	0.6194	0.027*
C19B	−0.03907 (11)	0.9669 (2)	0.59513 (14)	0.0251 (5)
H19B	−0.0316	1.0065	0.6400	0.030*
C20B	−0.09128 (11)	0.9886 (2)	0.53973 (15)	0.0278 (6)
H20B	−0.1185	1.0426	0.5483	0.033*
C21B	−0.10314 (10)	0.9319 (2)	0.47305 (14)	0.0240 (5)
H21B	−0.1382	0.9469	0.4370	0.029*
C22B	−0.06195 (10)	0.8508 (2)	0.45956 (13)	0.0205 (5)
C23B	−0.03295 (10)	0.7149 (2)	0.37602 (13)	0.0211 (5)

C24B	−0.12697 (11)	0.8197 (3)	0.33482 (15)	0.0321 (6)
H24D	−0.1287	0.7704	0.2926	0.048*
H24E	−0.1303	0.9109	0.3232	0.048*
H24F	−0.1579	0.7941	0.3512	0.048*
C25B	0.04245 (11)	0.4992 (3)	0.29093 (14)	0.0279 (6)
H25C	0.0067	0.5402	0.2621	0.034*
H25D	0.0640	0.4801	0.2589	0.034*
C26B	0.02830 (14)	0.3718 (3)	0.32003 (18)	0.0409 (7)
H26D	0.0633	0.3285	0.3474	0.061*
H26E	0.0068	0.3173	0.2804	0.061*
H26F	0.0059	0.3888	0.3507	0.061*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1A	0.0234 (3)	0.0189 (3)	0.0154 (3)	0.0000 (2)	0.0035 (2)	0.0017 (2)
O1A	0.0248 (9)	0.0242 (9)	0.0241 (10)	0.0042 (7)	−0.0022 (7)	0.0033 (7)
O2A	0.0388 (11)	0.0285 (9)	0.0190 (9)	−0.0065 (8)	0.0114 (8)	0.0000 (7)
O3A	0.0152 (8)	0.0215 (8)	0.0178 (8)	0.0034 (6)	0.0063 (6)	0.0045 (6)
O4A	0.0196 (8)	0.0301 (9)	0.0212 (9)	0.0017 (7)	0.0095 (7)	0.0018 (7)
N1A	0.0174 (9)	0.0177 (9)	0.0150 (9)	0.0015 (7)	0.0041 (8)	0.0006 (7)
N2A	0.0147 (9)	0.0170 (9)	0.0178 (10)	0.0000 (7)	0.0051 (8)	−0.0035 (7)
C1A	0.0175 (11)	0.0183 (10)	0.0165 (11)	0.0013 (8)	0.0054 (9)	−0.0008 (8)
C2A	0.0161 (10)	0.0128 (9)	0.0146 (10)	−0.0004 (8)	0.0059 (8)	−0.0002 (8)
C3A	0.0163 (10)	0.0135 (9)	0.0132 (10)	−0.0008 (8)	0.0050 (8)	−0.0003 (8)
C4A	0.0170 (11)	0.0193 (10)	0.0159 (11)	0.0050 (8)	0.0046 (9)	0.0026 (8)
C5A	0.0141 (10)	0.0155 (10)	0.0151 (10)	0.0032 (8)	0.0046 (8)	0.0011 (8)
C6A	0.0146 (10)	0.0153 (10)	0.0145 (11)	−0.0006 (8)	0.0029 (8)	−0.0040 (8)
C7A	0.0144 (10)	0.0137 (10)	0.0137 (10)	−0.0010 (8)	0.0030 (8)	−0.0024 (8)
C8A	0.0199 (11)	0.0161 (10)	0.0129 (10)	−0.0026 (8)	0.0021 (9)	−0.0025 (8)
C9A	0.0211 (12)	0.0254 (12)	0.0188 (12)	−0.0034 (9)	0.0079 (10)	−0.0052 (9)
C10A	0.0186 (11)	0.0210 (11)	0.0254 (13)	0.0016 (9)	0.0063 (10)	−0.0041 (9)
C11A	0.0176 (11)	0.0198 (11)	0.0179 (11)	−0.0022 (9)	−0.0008 (9)	−0.0022 (9)
C12A	0.0155 (11)	0.0233 (11)	0.0202 (12)	−0.0034 (9)	0.0040 (9)	0.0006 (9)
C13A	0.0143 (11)	0.0240 (12)	0.0229 (12)	0.0014 (9)	0.0035 (9)	−0.0020 (9)
C14A	0.0243 (13)	0.0224 (12)	0.0302 (14)	−0.0011 (10)	0.0021 (11)	0.0046 (10)
C15A	0.0191 (11)	0.0206 (11)	0.0223 (12)	0.0001 (9)	0.0086 (10)	0.0023 (9)
C16A	0.0277 (13)	0.0223 (11)	0.0193 (12)	−0.0008 (10)	0.0108 (10)	−0.0061 (9)
C17A	0.0161 (11)	0.0141 (10)	0.0146 (11)	−0.0011 (8)	0.0026 (9)	−0.0038 (8)
C18A	0.0203 (11)	0.0176 (11)	0.0171 (11)	−0.0016 (9)	0.0048 (9)	−0.0013 (8)
C19A	0.0259 (12)	0.0197 (11)	0.0155 (11)	0.0001 (9)	0.0010 (10)	0.0015 (9)
C20A	0.0219 (12)	0.0162 (10)	0.0193 (12)	0.0026 (9)	−0.0030 (9)	−0.0003 (9)
C21A	0.0167 (11)	0.0168 (11)	0.0213 (12)	0.0005 (8)	0.0018 (9)	−0.0039 (9)
C22A	0.0161 (10)	0.0137 (10)	0.0176 (11)	−0.0012 (8)	0.0028 (9)	−0.0037 (8)
C23A	0.0144 (10)	0.0174 (10)	0.0153 (11)	−0.0002 (8)	0.0028 (9)	−0.0033 (8)
C24A	0.0189 (12)	0.0300 (13)	0.0271 (13)	0.0034 (10)	0.0097 (10)	−0.0033 (10)
C25A	0.0213 (12)	0.0353 (14)	0.0226 (13)	0.0045 (10)	0.0086 (10)	0.0115 (10)
C26A	0.0419 (17)	0.0297 (15)	0.0414 (18)	−0.0121 (12)	0.0127 (14)	0.0107 (12)

S1B	0.0275 (3)	0.0224 (3)	0.0290 (3)	0.0038 (2)	0.0167 (3)	0.0031 (2)
O1B	0.0319 (10)	0.0307 (10)	0.0520 (13)	0.0133 (8)	0.0271 (10)	0.0111 (9)
O2B	0.0489 (13)	0.0402 (11)	0.0259 (10)	−0.0057 (9)	0.0207 (10)	−0.0033 (8)
O3B	0.0195 (8)	0.0271 (9)	0.0193 (9)	0.0065 (7)	0.0049 (7)	0.0003 (7)
O4B	0.0283 (10)	0.0481 (12)	0.0171 (9)	0.0069 (9)	0.0033 (8)	−0.0012 (8)
N1B	0.0234 (10)	0.0199 (10)	0.0229 (11)	0.0058 (8)	0.0115 (9)	0.0054 (8)
N2B	0.0148 (9)	0.0218 (10)	0.0241 (11)	0.0024 (8)	0.0031 (8)	0.0042 (8)
C1B	0.0219 (12)	0.0231 (12)	0.0277 (13)	0.0068 (9)	0.0099 (10)	0.0048 (10)
C2B	0.0173 (11)	0.0175 (10)	0.0224 (12)	0.0028 (8)	0.0060 (9)	0.0048 (9)
C3B	0.0187 (11)	0.0175 (10)	0.0191 (11)	0.0021 (8)	0.0066 (9)	0.0034 (9)
C4B	0.0243 (12)	0.0216 (11)	0.0204 (12)	0.0042 (9)	0.0102 (10)	0.0034 (9)
C5B	0.0193 (11)	0.0209 (11)	0.0203 (12)	0.0062 (9)	0.0059 (9)	0.0047 (9)
C6B	0.0163 (11)	0.0172 (10)	0.0200 (12)	0.0002 (8)	0.0050 (9)	0.0027 (8)
C7B	0.0182 (11)	0.0180 (11)	0.0221 (12)	0.0005 (8)	0.0087 (9)	0.0043 (9)
C8B	0.0200 (12)	0.0222 (12)	0.0329 (14)	0.0019 (9)	0.0138 (11)	0.0041 (10)
C9B	0.0212 (12)	0.0311 (14)	0.0384 (15)	0.0043 (10)	0.0146 (11)	0.0150 (11)
C10B	0.0237 (14)	0.0284 (14)	0.079 (2)	0.0085 (11)	0.0289 (15)	0.0227 (15)
C11B	0.0258 (15)	0.0222 (14)	0.102 (3)	−0.0040 (11)	0.0373 (18)	−0.0020 (15)
C12B	0.0214 (14)	0.0398 (17)	0.074 (2)	−0.0098 (12)	0.0193 (15)	−0.0147 (16)
C13B	0.0176 (12)	0.0326 (14)	0.0392 (16)	0.0010 (10)	0.0071 (11)	−0.0006 (12)
C14B	0.041 (2)	0.0249 (17)	0.218 (6)	−0.0077 (15)	0.064 (3)	−0.025 (2)
C15B	0.0220 (13)	0.0376 (15)	0.0214 (13)	0.0053 (11)	0.0010 (10)	0.0010 (11)
C16B	0.0378 (15)	0.0286 (13)	0.0240 (13)	0.0048 (11)	0.0136 (12)	0.0111 (10)
C17B	0.0200 (12)	0.0178 (11)	0.0232 (12)	−0.0005 (9)	0.0092 (10)	0.0023 (9)
C18B	0.0225 (12)	0.0198 (11)	0.0267 (13)	0.0001 (9)	0.0117 (10)	0.0043 (9)
C19B	0.0298 (13)	0.0223 (12)	0.0280 (14)	0.0015 (10)	0.0158 (11)	0.0006 (10)
C20B	0.0271 (13)	0.0206 (12)	0.0408 (16)	0.0043 (10)	0.0183 (12)	0.0029 (11)
C21B	0.0183 (11)	0.0223 (12)	0.0329 (14)	0.0028 (9)	0.0103 (10)	0.0063 (10)
C22B	0.0190 (11)	0.0175 (11)	0.0264 (13)	−0.0010 (9)	0.0094 (10)	0.0039 (9)
C23B	0.0199 (12)	0.0220 (11)	0.0219 (12)	0.0019 (9)	0.0079 (10)	0.0053 (9)
C24B	0.0230 (13)	0.0360 (15)	0.0311 (15)	0.0058 (11)	0.0010 (11)	0.0049 (12)
C25B	0.0289 (14)	0.0314 (14)	0.0238 (13)	0.0035 (11)	0.0093 (11)	−0.0031 (10)
C26B	0.0443 (18)	0.0349 (16)	0.0421 (18)	−0.0119 (13)	0.0127 (15)	−0.0107 (13)

Geometric parameters (Å, °)

S1A—O2A	1.4337 (18)	S1B—O2B	1.430 (2)
S1A—O1A	1.4342 (18)	S1B—O1B	1.4345 (19)
S1A—N1A	1.629 (2)	S1B—N1B	1.634 (2)
S1A—C8A	1.772 (2)	S1B—C8B	1.770 (3)
O3A—C6A	1.353 (3)	O3B—C6B	1.353 (3)
O3A—C5A	1.473 (3)	O3B—C5B	1.471 (3)
O4A—C23A	1.231 (3)	O4B—C23B	1.233 (3)
N1A—C1A	1.491 (3)	N1B—C1B	1.479 (3)
N1A—C4A	1.522 (3)	N1B—C4B	1.517 (3)
N2A—C23A	1.388 (3)	N2B—C23B	1.385 (3)
N2A—C22A	1.388 (3)	N2B—C22B	1.386 (3)
N2A—C24A	1.462 (3)	N2B—C24B	1.464 (3)
C1A—C2A	1.512 (3)	C1B—C2B	1.519 (3)

C1A—H1A	0.97	C1B—H1C	0.97
C1A—H1B	0.97	C1B—H1D	0.97
C2A—C5A	1.517 (3)	C2B—C5B	1.514 (3)
C2A—C3A	1.525 (3)	C2B—C3B	1.522 (3)
C2A—H2A	0.98	C2B—H2B	0.98
C3A—C7A	1.510 (3)	C3B—C7B	1.509 (3)
C3A—C4A	1.544 (3)	C3B—C4B	1.546 (3)
C3A—H3A	0.98	C3B—H3B	0.98
C4A—C25A	1.527 (3)	C4B—C25B	1.533 (4)
C4A—H4A	0.98	C4B—H4B	0.98
C5A—C15A	1.510 (3)	C5B—C15B	1.516 (4)
C5A—C16A	1.519 (3)	C5B—C16B	1.523 (3)
C6A—C7A	1.365 (3)	C6B—C7B	1.360 (3)
C6A—C17A	1.444 (3)	C6B—C17B	1.446 (3)
C7A—C23A	1.449 (3)	C7B—C23B	1.450 (3)
C8A—C9A	1.388 (3)	C8B—C13B	1.380 (4)
C8A—C13A	1.388 (3)	C8B—C9B	1.394 (3)
C9A—C10A	1.396 (3)	C9B—C10B	1.386 (4)
C9A—H9A	0.93	C9B—H9B	0.93
C10A—C11A	1.384 (3)	C10B—C11B	1.377 (5)
C10A—H10A	0.93	C10B—H10B	0.93
C11A—C12A	1.395 (3)	C11B—C12B	1.390 (5)
C11A—C14A	1.509 (3)	C11B—C14B	1.504 (4)
C12A—C13A	1.388 (3)	C12B—C13B	1.389 (4)
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—H14E	0.96
C14A—H14C	0.96	C14B—H14F	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
C17A—C18A	1.406 (3)	C17B—C22B	1.402 (3)
C17A—C22A	1.408 (3)	C17B—C18B	1.402 (3)
C18A—C19A	1.374 (3)	C18B—C19B	1.373 (3)
C18A—H18A	0.93	C18B—H18B	0.93
C19A—C20A	1.394 (3)	C19B—C20B	1.399 (4)
C19A—H19A	0.93	C19B—H19B	0.93
C20A—C21A	1.373 (3)	C20B—C21B	1.371 (4)
C20A—H20A	0.93	C20B—H20B	0.93
C21A—C22A	1.408 (3)	C21B—C22B	1.407 (3)
C21A—H21A	0.93	C21B—H21B	0.93
C24A—H24A	0.96	C24B—H24D	0.96
C24A—H24B	0.96	C24B—H24E	0.96
C24A—H24C	0.96	C24B—H24F	0.96
C25A—C26A	1.517 (4)	C25B—C26B	1.515 (4)

C25A—H25A	0.97	C25B—H25C	0.97
C25A—H25B	0.97	C25B—H25D	0.97
C26A—H26A	0.96	C26B—H26D	0.96
C26A—H26B	0.96	C26B—H26E	0.96
C26A—H26C	0.96	C26B—H26F	0.96
O2A—S1A—O1A	120.04 (11)	O2B—S1B—O1B	120.47 (12)
O2A—S1A—N1A	106.95 (10)	O2B—S1B—N1B	107.05 (11)
O1A—S1A—N1A	107.06 (10)	O1B—S1B—N1B	106.75 (11)
O2A—S1A—C8A	106.88 (11)	O2B—S1B—C8B	106.82 (12)
O1A—S1A—C8A	107.71 (11)	O1B—S1B—C8B	107.23 (12)
N1A—S1A—C8A	107.68 (10)	N1B—S1B—C8B	108.02 (11)
C6A—O3A—C5A	119.92 (16)	C6B—O3B—C5B	120.29 (18)
C1A—N1A—C4A	110.37 (17)	C1B—N1B—C4B	110.95 (17)
C1A—N1A—S1A	117.12 (15)	C1B—N1B—S1B	117.12 (16)
C4A—N1A—S1A	118.12 (14)	C4B—N1B—S1B	117.97 (15)
C23A—N2A—C22A	122.72 (18)	C23B—N2B—C22B	123.1 (2)
C23A—N2A—C24A	117.08 (19)	C23B—N2B—C24B	117.8 (2)
C22A—N2A—C24A	120.00 (19)	C22B—N2B—C24B	119.2 (2)
N1A—C1A—C2A	101.89 (17)	N1B—C1B—C2B	102.15 (18)
N1A—C1A—H1A	111.4	N1B—C1B—H1C	111.3
C2A—C1A—H1A	111.4	C2B—C1B—H1C	111.3
N1A—C1A—H1B	111.4	N1B—C1B—H1D	111.3
C2A—C1A—H1B	111.4	C2B—C1B—H1D	111.3
H1A—C1A—H1B	109.3	H1C—C1B—H1D	109.2
C1A—C2A—C5A	119.93 (18)	C5B—C2B—C1B	119.59 (19)
C1A—C2A—C3A	102.50 (17)	C5B—C2B—C3B	113.15 (19)
C5A—C2A—C3A	112.88 (18)	C1B—C2B—C3B	102.40 (19)
C1A—C2A—H2A	106.9	C5B—C2B—H2B	107.0
C5A—C2A—H2A	106.9	C1B—C2B—H2B	107.0
C3A—C2A—H2A	106.9	C3B—C2B—H2B	107.0
C7A—C3A—C2A	107.43 (17)	C7B—C3B—C2B	107.33 (19)
C7A—C3A—C4A	121.54 (18)	C7B—C3B—C4B	121.75 (19)
C2A—C3A—C4A	102.96 (17)	C2B—C3B—C4B	103.24 (18)
C7A—C3A—H3A	108.1	C7B—C3B—H3B	107.9
C2A—C3A—H3A	108.1	C2B—C3B—H3B	107.9
C4A—C3A—H3A	108.1	C4B—C3B—H3B	107.9
N1A—C4A—C25A	109.64 (18)	N1B—C4B—C25B	109.63 (19)
N1A—C4A—C3A	102.03 (16)	N1B—C4B—C3B	101.85 (18)
C25A—C4A—C3A	117.7 (2)	C25B—C4B—C3B	117.9 (2)
N1A—C4A—H4A	109.0	N1B—C4B—H4B	109.0
C25A—C4A—H4A	109.0	C25B—C4B—H4B	109.0
C3A—C4A—H4A	109.0	C3B—C4B—H4B	109.0
O3A—C5A—C15A	103.96 (17)	O3B—C5B—C2B	107.27 (18)
O3A—C5A—C2A	106.81 (16)	O3B—C5B—C15B	103.73 (19)
C15A—C5A—C2A	112.11 (19)	C2B—C5B—C15B	111.7 (2)
O3A—C5A—C16A	107.43 (18)	O3B—C5B—C16B	107.07 (19)
C15A—C5A—C16A	111.33 (18)	C2B—C5B—C16B	114.7 (2)
C2A—C5A—C16A	114.43 (18)	C15B—C5B—C16B	111.5 (2)
O3A—C6A—C7A	125.6 (2)	O3B—C6B—C7B	125.8 (2)

O3A—C6A—C17A	112.93 (18)	O3B—C6B—C17B	112.8 (2)
C7A—C6A—C17A	121.5 (2)	C7B—C6B—C17B	121.5 (2)
C6A—C7A—C23A	119.6 (2)	C6B—C7B—C23B	119.9 (2)
C6A—C7A—C3A	118.96 (19)	C6B—C7B—C3B	118.5 (2)
C23A—C7A—C3A	121.27 (19)	C23B—C7B—C3B	121.6 (2)
C9A—C8A—C13A	120.2 (2)	C13B—C8B—C9B	120.5 (2)
C9A—C8A—S1A	119.90 (17)	C13B—C8B—S1B	120.3 (2)
C13A—C8A—S1A	119.86 (17)	C9B—C8B—S1B	119.1 (2)
C8A—C9A—C10A	119.3 (2)	C10B—C9B—C8B	118.8 (3)
C8A—C9A—H9A	120.4	C10B—C9B—H9B	120.6
C10A—C9A—H9A	120.4	C8B—C9B—H9B	120.6
C11A—C10A—C9A	121.2 (2)	C11B—C10B—C9B	121.8 (3)
C11A—C10A—H10A	119.4	C11B—C10B—H10B	119.1
C9A—C10A—H10A	119.4	C9B—C10B—H10B	119.1
C10A—C11A—C12A	118.7 (2)	C10B—C11B—C12B	118.5 (3)
C10A—C11A—C14A	120.9 (2)	C10B—C11B—C14B	120.9 (3)
C12A—C11A—C14A	120.4 (2)	C12B—C11B—C14B	120.6 (4)
C13A—C12A—C11A	120.7 (2)	C13B—C12B—C11B	121.0 (3)
C13A—C12A—H12A	119.7	C13B—C12B—H12B	119.5
C11A—C12A—H12A	119.7	C11B—C12B—H12B	119.5
C8A—C13A—C12A	119.9 (2)	C8B—C13B—C12B	119.4 (3)
C8A—C13A—H13A	120.1	C8B—C13B—H13B	120.3
C12A—C13A—H13A	120.1	C12B—C13B—H13B	120.3
C11A—C14A—H14A	109.5	C11B—C14B—H14D	109.5
C11A—C14A—H14B	109.5	C11B—C14B—H14E	109.5
H14A—C14A—H14B	109.5	H14D—C14B—H14E	109.5
C11A—C14A—H14C	109.5	C11B—C14B—H14F	109.5
H14A—C14A—H14C	109.5	H14D—C14B—H14F	109.5
H14B—C14A—H14C	109.5	H14E—C14B—H14F	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
C18A—C17A—C22A	119.6 (2)	C22B—C17B—C18B	119.6 (2)
C18A—C17A—C6A	122.3 (2)	C22B—C17B—C6B	118.2 (2)
C22A—C17A—C6A	118.1 (2)	C18B—C17B—C6B	122.3 (2)
C19A—C18A—C17A	120.5 (2)	C19B—C18B—C17B	120.6 (2)
C19A—C18A—H18A	119.8	C19B—C18B—H18B	119.7
C17A—C18A—H18A	119.8	C17B—C18B—H18B	119.7
C18A—C19A—C20A	119.6 (2)	C18B—C19B—C20B	119.3 (2)
C18A—C19A—H19A	120.2	C18B—C19B—H19B	120.3

C20A—C19A—H19A	120.2	C20B—C19B—H19B	120.3
C21A—C20A—C19A	121.4 (2)	C21B—C20B—C19B	121.4 (2)
C21A—C20A—H20A	119.3	C21B—C20B—H20B	119.3
C19A—C20A—H20A	119.3	C19B—C20B—H20B	119.3
C20A—C21A—C22A	119.7 (2)	C20B—C21B—C22B	119.6 (2)
C20A—C21A—H21A	120.1	C20B—C21B—H21B	120.2
C22A—C21A—H21A	120.1	C22B—C21B—H21B	120.2
N2A—C22A—C17A	119.7 (2)	N2B—C22B—C17B	119.7 (2)
N2A—C22A—C21A	121.1 (2)	N2B—C22B—C21B	120.8 (2)
C17A—C22A—C21A	119.2 (2)	C17B—C22B—C21B	119.4 (2)
O4A—C23A—N2A	120.1 (2)	O4B—C23B—N2B	120.2 (2)
O4A—C23A—C7A	122.1 (2)	O4B—C23B—C7B	122.1 (2)
N2A—C23A—C7A	117.77 (19)	N2B—C23B—C7B	117.7 (2)
N2A—C24A—H24A	109.5	N2B—C24B—H24D	109.5
N2A—C24A—H24B	109.5	N2B—C24B—H24E	109.5
H24A—C24A—H24B	109.5	H24D—C24B—H24E	109.5
N2A—C24A—H24C	109.5	N2B—C24B—H24F	109.5
H24A—C24A—H24C	109.5	H24D—C24B—H24F	109.5
H24B—C24A—H24C	109.5	H24E—C24B—H24F	109.5
C26A—C25A—C4A	115.1 (2)	C26B—C25B—C4B	115.7 (2)
C26A—C25A—H25A	108.5	C26B—C25B—H25C	108.4
C4A—C25A—H25A	108.5	C4B—C25B—H25C	108.4
C26A—C25A—H25B	108.5	C26B—C25B—H25D	108.4
C4A—C25A—H25B	108.5	C4B—C25B—H25D	108.4
H25A—C25A—H25B	107.5	H25C—C25B—H25D	107.4
C25A—C26A—H26A	109.5	C25B—C26B—H26D	109.5
C25A—C26A—H26B	109.5	C25B—C26B—H26E	109.5
H26A—C26A—H26B	109.5	H26D—C26B—H26E	109.5
C25A—C26A—H26C	109.5	C25B—C26B—H26F	109.5
H26A—C26A—H26C	109.5	H26D—C26B—H26F	109.5
H26B—C26A—H26C	109.5	H26E—C26B—H26F	109.5
O2A—S1A—N1A—C1A	176.48 (15)	O2B—S1B—N1B—C1B	175.40 (17)
O1A—S1A—N1A—C1A	46.62 (18)	O1B—S1B—N1B—C1B	45.15 (19)
C8A—S1A—N1A—C1A	−68.96 (18)	C8B—S1B—N1B—C1B	−69.89 (19)
O2A—S1A—N1A—C4A	−47.70 (18)	O2B—S1B—N1B—C4B	−48.0 (2)
O1A—S1A—N1A—C4A	−177.56 (15)	O1B—S1B—N1B—C4B	−178.22 (17)
C8A—S1A—N1A—C4A	66.86 (18)	C8B—S1B—N1B—C4B	66.7 (2)
C4A—N1A—C1A—C2A	−22.5 (2)	C4B—N1B—C1B—C2B	−21.8 (2)
S1A—N1A—C1A—C2A	116.49 (16)	S1B—N1B—C1B—C2B	117.67 (17)
N1A—C1A—C2A—C5A	166.83 (18)	N1B—C1B—C2B—C5B	165.9 (2)
N1A—C1A—C2A—C3A	40.9 (2)	N1B—C1B—C2B—C3B	39.9 (2)
C1A—C2A—C3A—C7A	−174.14 (17)	C5B—C2B—C3B—C7B	56.4 (2)
C5A—C2A—C3A—C7A	55.5 (2)	C1B—C2B—C3B—C7B	−173.54 (18)
C1A—C2A—C3A—C4A	−44.7 (2)	C5B—C2B—C3B—C4B	−173.86 (18)
C5A—C2A—C3A—C4A	−175.14 (17)	C1B—C2B—C3B—C4B	−43.8 (2)
C1A—N1A—C4A—C25A	−130.1 (2)	C1B—N1B—C4B—C25B	−130.4 (2)
S1A—N1A—C4A—C25A	91.3 (2)	S1B—N1B—C4B—C25B	90.5 (2)
C1A—N1A—C4A—C3A	−4.6 (2)	C1B—N1B—C4B—C3B	−4.7 (2)
S1A—N1A—C4A—C3A	−143.16 (15)	S1B—N1B—C4B—C3B	−143.86 (16)

C7A—C3A—C4A—N1A	149.90 (19)	C7B—C3B—C4B—N1B	149.9 (2)
C2A—C3A—C4A—N1A	29.8 (2)	C2B—C3B—C4B—N1B	29.5 (2)
C7A—C3A—C4A—C25A	−90.1 (3)	C7B—C3B—C4B—C25B	−90.2 (3)
C2A—C3A—C4A—C25A	149.78 (19)	C2B—C3B—C4B—C25B	149.5 (2)
C6A—O3A—C5A—C15A	151.29 (18)	C6B—O3B—C5B—C2B	28.9 (3)
C6A—O3A—C5A—C2A	32.6 (2)	C6B—O3B—C5B—C15B	147.3 (2)
C6A—O3A—C5A—C16A	−90.6 (2)	C6B—O3B—C5B—C16B	−94.7 (2)
C1A—C2A—C5A—O3A	−179.95 (18)	C1B—C2B—C5B—O3B	−177.9 (2)
C3A—C2A—C5A—O3A	−59.0 (2)	C3B—C2B—C5B—O3B	−57.1 (2)
C1A—C2A—C5A—C15A	66.8 (3)	C1B—C2B—C5B—C15B	69.1 (3)
C3A—C2A—C5A—C15A	−172.27 (18)	C3B—C2B—C5B—C15B	−170.18 (19)
C1A—C2A—C5A—C16A	−61.2 (3)	C1B—C2B—C5B—C16B	−59.1 (3)
C3A—C2A—C5A—C16A	59.7 (2)	C3B—C2B—C5B—C16B	61.7 (3)
C5A—O3A—C6A—C7A	−4.6 (3)	C5B—O3B—C6B—C7B	−1.8 (3)
C5A—O3A—C6A—C17A	176.12 (18)	C5B—O3B—C6B—C17B	178.79 (19)
O3A—C6A—C7A—C23A	175.99 (19)	O3B—C6B—C7B—C23B	179.2 (2)
C17A—C6A—C7A—C23A	−4.8 (3)	C17B—C6B—C7B—C23B	−1.5 (3)
O3A—C6A—C7A—C3A	0.6 (3)	O3B—C6B—C7B—C3B	1.0 (3)
C17A—C6A—C7A—C3A	179.80 (19)	C17B—C6B—C7B—C3B	−179.7 (2)
C2A—C3A—C7A—C6A	−25.3 (3)	C2B—C3B—C7B—C6B	−27.3 (3)
C4A—C3A—C7A—C6A	−143.2 (2)	C4B—C3B—C7B—C6B	−145.7 (2)
C2A—C3A—C7A—C23A	159.40 (19)	C2B—C3B—C7B—C23B	154.5 (2)
C4A—C3A—C7A—C23A	41.5 (3)	C4B—C3B—C7B—C23B	36.2 (3)
O2A—S1A—C8A—C9A	20.4 (2)	O2B—S1B—C8B—C13B	−158.5 (2)
O1A—S1A—C8A—C9A	150.68 (19)	O1B—S1B—C8B—C13B	−28.1 (2)
N1A—S1A—C8A—C9A	−94.2 (2)	N1B—S1B—C8B—C13B	86.6 (2)
O2A—S1A—C8A—C13A	−161.33 (19)	O2B—S1B—C8B—C9B	23.2 (2)
O1A—S1A—C8A—C13A	−31.1 (2)	O1B—S1B—C8B—C9B	153.66 (19)
N1A—S1A—C8A—C13A	84.1 (2)	N1B—S1B—C8B—C9B	−91.6 (2)
C13A—C8A—C9A—C10A	−0.5 (4)	C13B—C8B—C9B—C10B	−1.3 (4)
S1A—C8A—C9A—C10A	177.74 (18)	S1B—C8B—C9B—C10B	176.99 (19)
C8A—C9A—C10A—C11A	0.0 (4)	C8B—C9B—C10B—C11B	−0.4 (4)
C9A—C10A—C11A—C12A	0.4 (4)	C9B—C10B—C11B—C12B	1.4 (4)
C9A—C10A—C11A—C14A	−177.1 (2)	C9B—C10B—C11B—C14B	−175.7 (3)
C10A—C11A—C12A—C13A	−0.3 (4)	C10B—C11B—C12B—C13B	−0.8 (5)
C14A—C11A—C12A—C13A	177.2 (2)	C14B—C11B—C12B—C13B	176.3 (3)
C9A—C8A—C13A—C12A	0.6 (4)	C9B—C8B—C13B—C12B	1.9 (4)
S1A—C8A—C13A—C12A	−177.62 (18)	S1B—C8B—C13B—C12B	−176.4 (2)
C11A—C12A—C13A—C8A	−0.2 (4)	C11B—C12B—C13B—C8B	−0.9 (4)
O3A—C6A—C17A—C18A	−0.1 (3)	O3B—C6B—C17B—C22B	−179.0 (2)
C7A—C6A—C17A—C18A	−179.4 (2)	C7B—C6B—C17B—C22B	1.6 (3)
O3A—C6A—C17A—C22A	178.89 (18)	O3B—C6B—C17B—C18B	1.9 (3)
C7A—C6A—C17A—C22A	−0.4 (3)	C7B—C6B—C17B—C18B	−177.5 (2)
C22A—C17A—C18A—C19A	0.0 (3)	C22B—C17B—C18B—C19B	0.6 (3)
C6A—C17A—C18A—C19A	179.0 (2)	C6B—C17B—C18B—C19B	179.6 (2)
C17A—C18A—C19A—C20A	−0.4 (3)	C17B—C18B—C19B—C20B	0.3 (4)
C18A—C19A—C20A—C21A	0.8 (4)	C18B—C19B—C20B—C21B	−0.4 (4)
C19A—C20A—C21A—C22A	−0.7 (3)	C19B—C20B—C21B—C22B	−0.4 (4)
C23A—N2A—C22A—C17A	3.2 (3)	C23B—N2B—C22B—C17B	0.4 (3)

C24A—N2A—C22A—C17A	178.0 (2)	C24B—N2B—C22B—C17B	179.3 (2)
C23A—N2A—C22A—C21A	−176.5 (2)	C23B—N2B—C22B—C21B	179.9 (2)
C24A—N2A—C22A—C21A	−1.6 (3)	C24B—N2B—C22B—C21B	−1.2 (3)
C18A—C17A—C22A—N2A	−179.6 (2)	C18B—C17B—C22B—N2B	178.1 (2)
C6A—C17A—C22A—N2A	1.4 (3)	C6B—C17B—C22B—N2B	−1.0 (3)
C18A—C17A—C22A—C21A	0.1 (3)	C18B—C17B—C22B—C21B	−1.4 (3)
C6A—C17A—C22A—C21A	−179.0 (2)	C6B—C17B—C22B—C21B	179.5 (2)
C20A—C21A—C22A—N2A	180.0 (2)	C20B—C21B—C22B—N2B	−178.1 (2)
C20A—C21A—C22A—C17A	0.3 (3)	C20B—C21B—C22B—C17B	1.3 (3)
C22A—N2A—C23A—O4A	171.4 (2)	C22B—N2B—C23B—O4B	179.4 (2)
C24A—N2A—C23A—O4A	−3.6 (3)	C24B—N2B—C23B—O4B	0.5 (3)
C22A—N2A—C23A—C7A	−8.3 (3)	C22B—N2B—C23B—C7B	−0.3 (3)
C24A—N2A—C23A—C7A	176.72 (19)	C24B—N2B—C23B—C7B	−179.2 (2)
C6A—C7A—C23A—O4A	−170.7 (2)	C6B—C7B—C23B—O4B	−178.9 (2)
C3A—C7A—C23A—O4A	4.6 (3)	C3B—C7B—C23B—O4B	−0.7 (3)
C6A—C7A—C23A—N2A	9.0 (3)	C6B—C7B—C23B—N2B	0.8 (3)
C3A—C7A—C23A—N2A	−175.71 (19)	C3B—C7B—C23B—N2B	179.0 (2)
N1A—C4A—C25A—C26A	77.8 (3)	N1B—C4B—C25B—C26B	82.2 (3)
C3A—C4A—C25A—C26A	−38.1 (3)	C3B—C4B—C25B—C26B	−33.6 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C25A—H25A···O4A	0.97	2.27	2.915 (3)	123
C25A—H25B···O2A	0.97	2.53	3.182 (3)	125
C25B—H25C···O4B	0.97	2.29	2.916 (4)	121
C25B—H25D···O2B	0.97	2.52	3.170 (4)	124
C10A—H10A···O4A^{i}	0.93	2.41	3.279 (3)	155
C24A—H24A···O2A^{i}	0.96	2.58	3.466 (3)	153
C10B—H10B···O4B^{ii}	0.93	2.36	3.273 (4)	167
C24B—H24E···O2B^{ii}	0.96	2.49	3.406 (4)	159
C16A—H16C···Cg1^{iii}	0.96	2.81	3.416 (2)	122
C20A—H20A···Cg2^{iv}	0.93	2.87	3.631 (3)	140
C16B—H16D···Cg4^{v}	0.96	2.90	3.612 (3)	131
C20B—H20B···Cg5^{vi}	0.93	2.82	3.589 (3)	141
C12A—H12A···Cg5^{vii}	0.93	2.87	3.782 (3)	166

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

Fig. 1

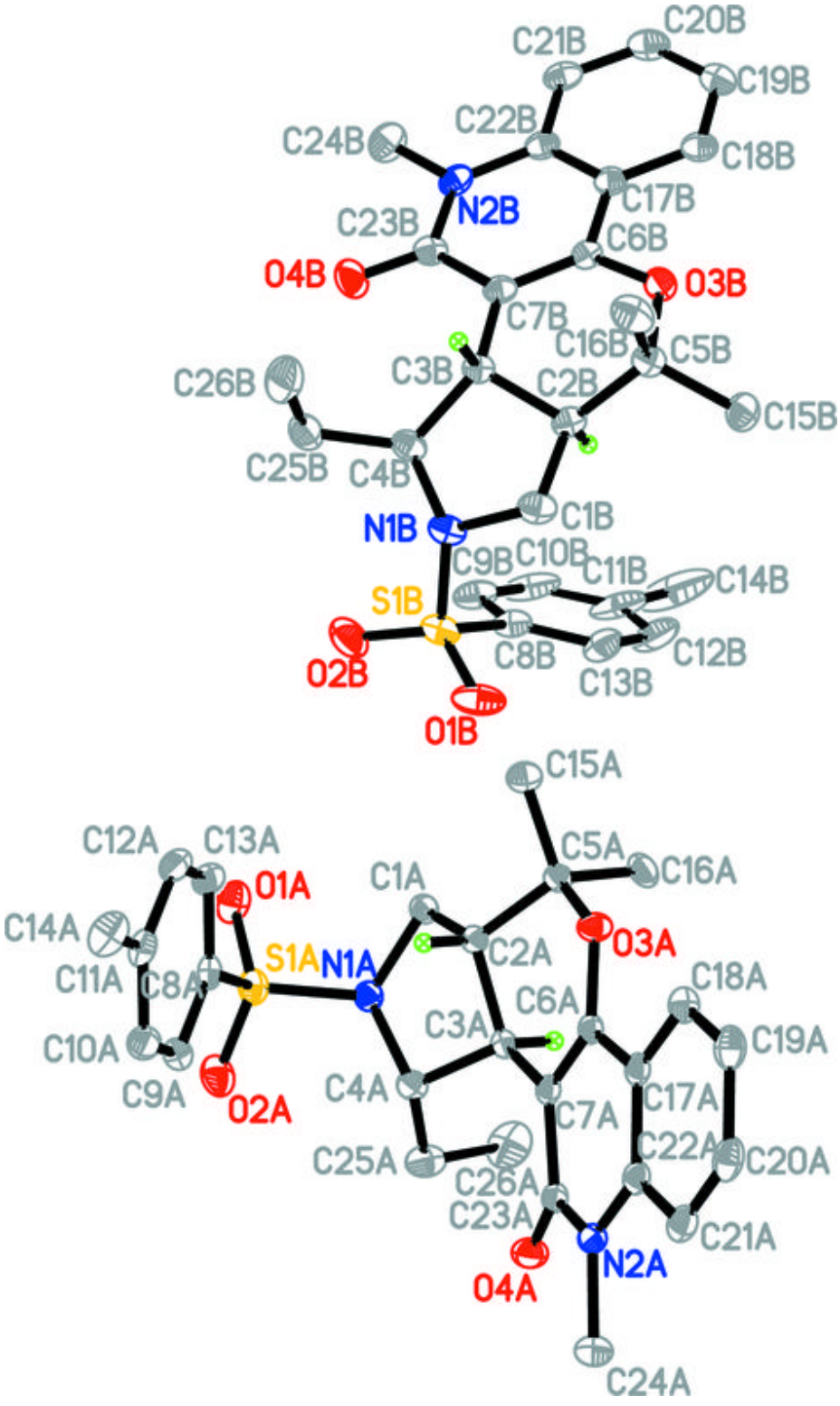
C20B
C21B
C19B
C22B
C24B
C18B
N2B
C17B
C23B
C6B
O4B
O3B
C7B
C16B
C5B
C3B
C26B
C2B
C15B
C25B
C4B
N1B
C1B
C9B
C10B
C11B
C14B
S1B
C8B
C12B
O2B
C13B
O1B
C15A
C12A
C13A
C5A
C16A
O1A
C1A
C14A
O3A
S1A
N1A
C2A
C11A
C8A
C18A
C6A
C3A
C10A
C19A
C9A
C4A
C17A
O2A
C7A
C25A
C22A
C20A
C26A
C23A
C21A
O4A
N2A
C24A

Fig. 2

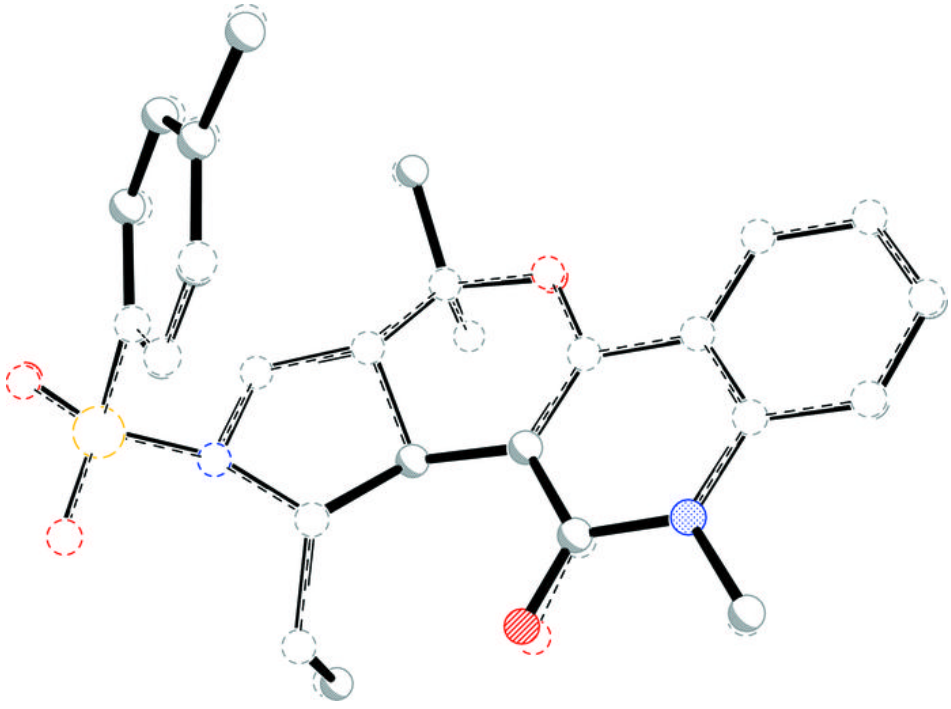

Fig. 3