Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

7-Chloro-3-ethyl-9,9-dimethyl-2-tosyl-2,3,3a,4,9,9a-hexahydro-1*H*-pyrrolo[3,4-*b*]quinoline

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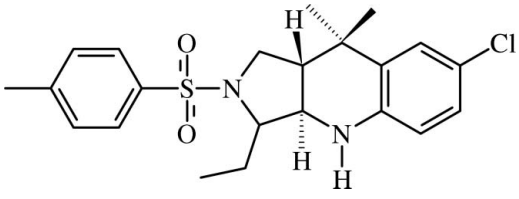
Received 12 November 2007; accepted 20 November 2007

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.060; wR factor = 0.195; data-to-parameter ratio = 35.9.

The asymmetric unit of the title compound, $C_{22}H_{27}ClN_2O_2S$, consists of two independent molecules, *A* and *B*, with similar conformations. In both molecules, the pyrrolidine rings adopt twist conformations and the tetrahydropyridine rings have half-chair conformations; these rings are *trans*-fused. In molecule *A*, the tosyl group is attached equatorially to the pyrrolidine ring, whereas in molecule *B* it is in a biaxial position. In both molecules, the sulfonyl groups have distorted tetrahedral geometries. Molecules *A* and *B* are linked into a two-dimensional network parallel to the *ab* plane by N—H···O and C—H···O hydrogen bonds, and C—H···π interactions.

Related literature

For biological activities of pyrrolo[3,4-*b*]quinoline derivatives, see: Anzini *et al.* (1990, 1992); Crenshaw *et al.* (1976); Fujita *et al.* (1996); Xiao *et al.* (2006). For ring puckering parameters, see: Cremer & Pople (1975). For asymmetry parameters, see: Duax *et al.* (1976).



Experimental

Crystal data

$C_{22}H_{27}ClN_2O_2S$
M_r = 418.97
Triclinic, $P\overline{1}$
a = 11.4284 (2) Å
b = 13.8093 (2) Å
c = 14.5937 (2) Å
α = 109.911 (1)°
β = 98.168 (1)°
γ = 92.601 (1)°
V = 2132.60 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.30 mm^{-1}
T = 100.0 (1) K
0.35 × 0.21 × 0.16 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.841, T_{max} = 0.955
44677 measured reflections
18502 independent reflections
11189 reflections with $I > 2\sigma(I)$
R_{int} = 0.053

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.195
S = 1.01
18502 reflections
515 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.81 e Å^{-3}
$\Delta\rho_{min}$ = −0.67 e Å^{-3}

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

*Cg*1 and *Cg*2 are the centroids of the rings C4*B*–C9*B* and C12*A*–C17*A*, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2*A*—H1N···O1*B*^{i}	0.86 (3)	2.44 (2)	3.285 (2)	167 (2)
N2*B*—H2N···O1*A*^{ii}	0.92 (3)	2.29 (2)	3.188 (2)	165 (2)
C8*A*—H8*A*···O1*B*^{iii}	0.93	2.49	3.327 (2)	149
C21*A*—H21*B*···O1*B*^{i}	0.97	2.52	3.447 (3)	159
C1*A*—H1*A*···*Cg*1	0.97	2.92	3.760 (2)	145
C14*A*—H14*A*···*Cg*1^{iii}	0.93	3.00	3.876 (2)	158
C22*B*—H22*D*···*Cg*2^{ii}	0.97	2.84	3.558 (2)	133
C13*A*—H13*A*···O2*A*^{iv}	0.93	2.52	3.294 (2)	141
C21*A*—H21*A*···O2*A*	0.97	2.50	3.101 (3)	120
C21*B*—H21*D*···O2*B*	0.97	2.57	3.158 (1)	119

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

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

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: SJ2437).

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  doi:10.1107/S1600536807061351

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supplementary materials

Acta Cryst. (2007). E**63**, o4912-o4913 [**doi:10.1107/S1600536807061351**]

7-Chloro-3-ethyl-9,9-dimethyl-2-tosyl-2,3,3a,4,9,9a-hexahydro-1*H*-pyrrolo[3,4-*b*]quinoline

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

Comment

Pyrrolo[3,4-*b*]quinoline derivatives exhibit cytotoxic (Xiao *et al.*, 2006) and antibacterial (Fujita *et al.*, 1996) activities. The derivatives are also found to have interferon inducing activities (Crenshaw *et al.*, 1976) and the ability to bind benzodiazepine receptors (Anzini *et al.*, 1990, 1992). We report here the crystal structure of the title compound, a pyrrolo[3,4-*b*]quinoline derivative.

The asymmetric unit of the title compound contains two independent molecules, *A* and *B*, with almost 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 0.254 Å.

The pyrrolidine rings in each of the molecule *A* and *B* adopt a twist conformation, with local twofold rotation axes passing through atoms N1 and the midpoints of the C2—C10 bonds. The relevant asymmetry parameters (Duax *et al.*, 1976) are ΔC_2[C2—C10] = 9.0 (2)° for molecule *A* and 10.2 (2)° for molecule *B*; the puckering parameters q_2 and φ (Cremer & Pople, 1975) are 0.419 (2) Å and 262.9 (3)° for molecule *A*, and 0.445 (2) Å and 82.2 (2)° for molecule *B*. The tosyl group is equatorially attached to the pyrrolidine ring in molecule *A* and in molecule *B* it is in a biaxial position.

In each of the independent molecules, the tetrahydropyridine rings adopt half-chair conformations, with local pseudo-twofold axes running through the midpoints of the C4—C9 and C2—C10 bonds. The puckering parameters Q, θ and φ, and the smallest displacement asymmetry parameters ΔC_2[C4—C9] for the molecules *A*/*B* are 0.500 (2)/0.475 (2) Å, 46.7 (2)/135.5 (2)°, 273.0 (3)/91.9 (3)° and 5.5 (2)/5.0 (2)°.

In both molecules, the pyrrolidine rings are *trans*-fused to the tetrahydropyridine rings, and the sulfonyl groups have distorted tetrahedral geometries. The dihedral angles between the C4–C9 and C12–C17 benzene rings are 77.61 (9)° in molecule *A* and 62.90 (9)° in molecule *B*.

Molecules *A* and *B* are linked *via* N—H···O hydrogen bonds. The N—H···O and C—H···O hydrogen bonds, and C—H···π interactions (Table 1) involving the C4B–C9B (centroid *Cg*1) and C12A–C17 (centroid *Cg*2) rings link the molecules *A* and *B* into a two-dimensional network (Fig. 3) parallel to the *ab* plane.

Experimental

$InCl_3$ (20 mol%) was added to a mixture of 2-[*N*-(3-methylbut-2-enyl)-*N*-tosylamino]butanal (1 mmol) and 4-chloroaniline (1 mmol) in acetonitrile (2o ml). The reaction mixture was stirred at room temperature for 30 min. On completion of the reaction, as indicated by TLC, the mixture was quenched with water and extracted with ethyl acetate. The organic layer was washed with brine and dried over Na_2SO_4. The solvent was evaporated *in vacuo* and the crude product was chromatographed using a hexane–ethyl acetate (8.5:1.5 *v*/*v*) mixture to obtain the title compound. The compound was recrystallized from ethyl acetate solution by slow evaporation.

Refinement

N-bound H atoms were located from a difference map and refined freely. The remaining H atoms were positioned geometrically (C—H = 0.93–0.98 Å) and allowed to ride on their parent atoms, with 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. A search for solvent-accessible voids in the crystal using *PLATON* (Spek, 2003) showed a potential solvent volume of 97 $Å^3$ and subsequent application of SQUEEZE procedures showed two voids each with a solvent-accessible volume of 49 $Å^3$. The number of electrons found in each voids is 4. This indicates that the void is only partially occupied and that the original contents had probably disappeared by the time the crystal was used for data collection, without collapsing the structure. The final cycles of refinement was carried out using the original data and solvent free data was not used.

Figures

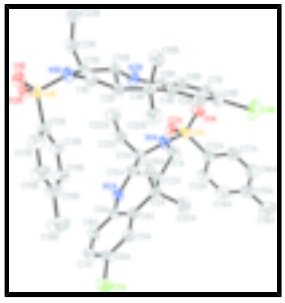


Fig. 1. The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 80% probability level. H atoms have been omitted for clarity.

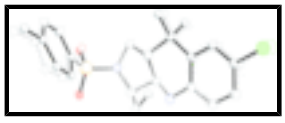


Fig. 2. Fit of molecule A (dashed lines) on molecule B (solid lines). H atoms have been omitted for clarity.

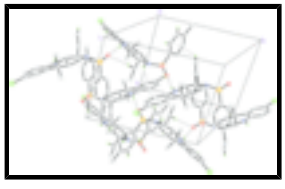


Fig. 3. Part of the two-dimensional network in the title compound. Dashed and dotted lines indicate N/C—H···O and C—H···π interactions, respectively. For the sake of clarity, H atoms not involved in the interactions have been omitted.

7-Chloro-3-ethyl-9,9-dimethyl-2-tosyl-2,3,3a,4,9,9a-hexahydro- 1*H*-pyrrolo[3,4-*b*]quinoline

Crystal data

$C_{22}H_{27}ClN_2O_2S$	$Z = 4$
$M_r = 418.97$	$F_{000} = 888$
Triclinic, $P\overline{1}$	$D_x = 1.305$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 11.4284$ (2) Å	Cell parameters from 6353 reflections
$b = 13.8093$ (2) Å	$\theta = 2.5$–$33.5°$
$c = 14.5937$ (2) Å	$\mu = 0.30$ mm^{-1}
$\alpha = 109.911$ (1)°	$T = 100.0$ (1) K

β = 98.168 (1)º	Block, colourless
γ = 92.601 (1)º	0.35 × 0.21 × 0.16 mm
V = 2132.60 (6) Å^3	

Data collection

Bruker APEXII CCD area-detector diffractometer	18502 independent reflections
Radiation source: fine-focus sealed tube	11189 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.053
Detector resolution: 8.33 pixels mm^{-1}	θ_{max} = 34.9º
T = 100.0(1) K	θ_{min} = 1.5º
ω scans	h = −18→18
Absorption correction: multi-scan (SADABS; Bruker, 2005)	k = −22→22
T_{min} = 0.841, T_{max} = 0.955	l = −23→21
44677 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
$R[F^2 > 2\sigma(F^2)]$ = 0.060	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.195	$w = 1/[\sigma^2(F_o^2) + (0.0989P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.01	$(\Delta/\sigma)_{max}$ = 0.001
18502 reflections	$\Delta\rho_{max}$ = 0.81 e Å^{-3}
515 parameters	$\Delta\rho_{min}$ = −0.67 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. The low-temparture data was collected with the Oxford Cyrosystem Cobra low-temperature attachment.

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1A	0.03018 (4)	−0.28932 (3)	0.51290 (3)	0.02648 (11)
S1A	0.21131 (4)	0.47964 (3)	0.90071 (3)	0.01826 (9)
O1A	0.31447 (11)	0.53422 (10)	0.88798 (10)	0.0220 (3)
O2A	0.17295 (12)	0.51397 (10)	0.99506 (9)	0.0223 (3)
N1A	0.23679 (14)	0.36009 (12)	0.87657 (11)	0.0203 (3)
N2A	0.10003 (13)	0.10860 (12)	0.85118 (11)	0.0181 (3)
H1N	0.107 (2)	0.0963 (19)	0.9055 (18)	0.028 (6)*
C1A	0.25764 (17)	0.29773 (14)	0.77589 (13)	0.0209 (3)
H1A	0.3404	0.2849	0.7759	0.025*
H1B	0.2341	0.3317	0.7289	0.025*
C2A	0.17823 (15)	0.19813 (13)	0.75292 (12)	0.0176 (3)
H2A	0.0960	0.2119	0.7364	0.021*
C3A	0.20094 (15)	0.10001 (13)	0.67079 (12)	0.0175 (3)
C4A	0.13319 (14)	0.00765 (13)	0.68351 (12)	0.0165 (3)
C5A	0.11398 (15)	−0.08803 (14)	0.60533 (13)	0.0188 (3)
H5A	0.1416	−0.0942	0.5468	0.023*
C6A	0.05469 (16)	−0.17335 (14)	0.61387 (13)	0.0214 (3)
C7A	0.01468 (16)	−0.16761 (14)	0.70034 (14)	0.0216 (3)
H7A	−0.0242	−0.2255	0.7058	0.026*
C8A	0.03339 (16)	−0.07384 (14)	0.77911 (14)	0.0202 (3)
H8A	0.0075	−0.0695	0.8379	0.024*
C9A	0.09096 (15)	0.01456 (13)	0.77120 (12)	0.0167 (3)
C10A	0.19221 (15)	0.18581 (13)	0.85341 (12)	0.0172 (3)
H10A	0.2705	0.1633	0.8683	0.021*
C11A	0.18479 (16)	0.29432 (14)	0.92669 (13)	0.0196 (3)
H11A	0.1013	0.3062	0.9297	0.024*
C12A	0.09332 (16)	0.48643 (13)	0.81127 (13)	0.0196 (3)
C13A	−0.02309 (16)	0.47016 (15)	0.82435 (14)	0.0228 (4)
H13A	−0.0387	0.4515	0.8772	0.027*
C14A	−0.11566 (17)	0.48205 (16)	0.75792 (15)	0.0270 (4)
H14A	−0.1936	0.4704	0.7662	0.032*
C15A	−0.09388 (18)	0.51126 (15)	0.67850 (15)	0.0260 (4)
C16A	0.02343 (18)	0.52595 (15)	0.66637 (14)	0.0249 (4)
H16A	0.0391	0.5442	0.6133	0.030*
C17A	0.11785 (17)	0.51390 (14)	0.73200 (13)	0.0219 (3)
H17A	0.1958	0.5240	0.7231	0.026*
C18A	−0.1946 (2)	0.52619 (19)	0.60841 (17)	0.0381 (5)
H18A	−0.1689	0.5775	0.5828	0.057*
H18B	−0.2597	0.5487	0.6427	0.057*
H18C	−0.2197	0.4619	0.5549	0.057*
C19A	0.33333 (16)	0.08292 (15)	0.67679 (15)	0.0247 (4)
H19A	0.3767	0.1400	0.6690	0.037*
H19B	0.3429	0.0199	0.6252	0.037*
H19C	0.3631	0.0782	0.7399	0.037*
C20A	0.15501 (19)	0.10988 (16)	0.57064 (14)	0.0259 (4)

H20A	0.1986	0.1679	0.5647	0.039*
H20B	0.0722	0.1201	0.5663	0.039*
H20C	0.1655	0.0478	0.5183	0.039*
C21A	0.25225 (18)	0.31623 (15)	1.03089 (14)	0.0246 (4)
H21A	0.2408	0.3857	1.0721	0.030*
H21B	0.2184	0.2685	1.0581	0.030*
C22A	0.38466 (18)	0.30659 (17)	1.03574 (16)	0.0299 (4)
H22A	0.4212	0.3214	1.1031	0.045*
H22B	0.4195	0.3548	1.0105	0.045*
H22C	0.3971	0.2374	0.9966	0.045*
Cl1B	0.47867 (5)	0.41939 (4)	0.55983 (4)	0.03280 (12)
S1B	0.74422 (4)	−0.03863 (3)	0.93978 (3)	0.01735 (9)
O1B	0.84439 (11)	−0.09847 (10)	0.92531 (10)	0.0213 (3)
O2B	0.70692 (11)	−0.00750 (10)	1.03451 (9)	0.0209 (3)
N1B	0.77511 (13)	0.06575 (11)	0.91748 (11)	0.0188 (3)
N2B	0.62984 (13)	0.28789 (12)	0.89959 (11)	0.0183 (3)
H2N	0.631 (2)	0.3406 (19)	0.9591 (18)	0.028 (6)*
C1B	0.78402 (16)	0.05627 (14)	0.81384 (13)	0.0194 (3)
H1C	0.7607	−0.0140	0.7684	0.023*
H1D	0.8639	0.0777	0.8083	0.023*
C2B	0.69617 (15)	0.13041 (13)	0.79504 (12)	0.0166 (3)
H2B	0.6159	0.0976	0.7877	0.020*
C3B	0.69986 (15)	0.16655 (14)	0.70689 (12)	0.0181 (3)
C4B	0.63027 (15)	0.26243 (14)	0.72451 (13)	0.0180 (3)
C5B	0.59119 (16)	0.29551 (15)	0.64625 (13)	0.0216 (3)
H5B	0.6056	0.2581	0.5833	0.026*
C6B	0.53138 (17)	0.38303 (15)	0.66045 (13)	0.0221 (3)
C7B	0.51099 (16)	0.44240 (15)	0.75307 (14)	0.0217 (3)
H7B	0.4729	0.5023	0.7623	0.026*
C8B	0.54853 (16)	0.41088 (14)	0.83191 (13)	0.0200 (3)
H8B	0.5359	0.4506	0.8948	0.024*
C9B	0.60504 (14)	0.32051 (13)	0.81907 (12)	0.0170 (3)
C10B	0.72086 (15)	0.21830 (13)	0.89397 (12)	0.0175 (3)
H10B	0.7985	0.2559	0.9017	0.021*
C11B	0.72455 (16)	0.16433 (13)	0.97009 (13)	0.0184 (3)
H11B	0.6432	0.1479	0.9783	0.022*
C12B	0.62353 (16)	−0.11225 (14)	0.84972 (13)	0.0189 (3)
C13B	0.50983 (16)	−0.08033 (15)	0.85445 (13)	0.0213 (3)
H13B	0.4980	−0.0193	0.9033	0.026*
C14B	0.41474 (16)	−0.14021 (15)	0.78585 (14)	0.0229 (4)
H14B	0.3391	−0.1183	0.7882	0.028*
C15B	0.43039 (17)	−0.23314 (16)	0.71312 (14)	0.0259 (4)
C16B	0.54457 (18)	−0.26339 (16)	0.70900 (14)	0.0283 (4)
H16B	0.5561	−0.3249	0.6606	0.034*
C17B	0.64184 (17)	−0.20334 (15)	0.77597 (14)	0.0243 (4)
H17B	0.7180	−0.2236	0.7717	0.029*
C18B	0.3257 (2)	−0.29909 (19)	0.64125 (17)	0.0372 (5)
H18D	0.3452	−0.3690	0.6143	0.056*
H18E	0.3059	−0.2726	0.5887	0.056*

H18F	0.2590	−0.2979	0.6747	0.056*
C19B	0.82765 (16)	0.19621 (15)	0.69704 (14)	0.0227 (3)
H19D	0.8716	0.1368	0.6860	0.034*
H19E	0.8651	0.2503	0.7567	0.034*
H19F	0.8259	0.2200	0.6423	0.034*
C20B	0.64319 (17)	0.07747 (15)	0.61165 (13)	0.0236 (4)
H20D	0.6886	0.0192	0.6029	0.035*
H20E	0.6423	0.0998	0.5561	0.035*
H20F	0.5633	0.0579	0.6166	0.035*
C21B	0.79862 (16)	0.22399 (14)	1.07127 (13)	0.0204 (3)
H21C	0.7635	0.2876	1.1008	0.024*
H21D	0.7943	0.1830	1.1133	0.024*
C22B	0.92898 (17)	0.25125 (15)	1.07013 (14)	0.0242 (4)
H22D	0.9688	0.2884	1.1364	0.036*
H22E	0.9347	0.2936	1.0304	0.036*
H22F	0.9656	0.1889	1.0429	0.036*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1A	0.0348 (2)	0.0154 (2)	0.0244 (2)	−0.00120 (17)	−0.00016 (17)	0.00328 (16)
S1A	0.0219 (2)	0.01295 (18)	0.01929 (19)	0.00118 (15)	0.00553 (15)	0.00415 (15)
O1A	0.0227 (6)	0.0168 (6)	0.0256 (6)	0.0004 (5)	0.0060 (5)	0.0058 (5)
O2A	0.0299 (7)	0.0167 (6)	0.0193 (6)	0.0031 (5)	0.0073 (5)	0.0038 (5)
N1A	0.0279 (8)	0.0138 (7)	0.0207 (7)	0.0023 (6)	0.0090 (6)	0.0057 (5)
N2A	0.0217 (7)	0.0164 (7)	0.0169 (6)	−0.0001 (5)	0.0050 (5)	0.0062 (5)
C1A	0.0272 (8)	0.0147 (8)	0.0205 (8)	−0.0006 (6)	0.0079 (6)	0.0046 (6)
C2A	0.0197 (7)	0.0152 (7)	0.0187 (7)	0.0019 (6)	0.0052 (6)	0.0064 (6)
C3A	0.0195 (7)	0.0153 (7)	0.0167 (7)	0.0008 (6)	0.0033 (6)	0.0045 (6)
C4A	0.0162 (7)	0.0144 (7)	0.0193 (7)	0.0031 (6)	0.0032 (6)	0.0060 (6)
C5A	0.0202 (8)	0.0171 (8)	0.0188 (7)	0.0022 (6)	0.0022 (6)	0.0062 (6)
C6A	0.0237 (8)	0.0156 (8)	0.0211 (8)	−0.0005 (6)	0.0003 (6)	0.0030 (6)
C7A	0.0235 (8)	0.0160 (8)	0.0250 (8)	−0.0016 (6)	0.0030 (6)	0.0076 (7)
C8A	0.0213 (8)	0.0183 (8)	0.0237 (8)	0.0020 (6)	0.0057 (6)	0.0101 (7)
C9A	0.0177 (7)	0.0141 (7)	0.0180 (7)	0.0011 (6)	0.0017 (6)	0.0059 (6)
C10A	0.0187 (7)	0.0149 (7)	0.0177 (7)	0.0004 (6)	0.0040 (6)	0.0053 (6)
C11A	0.0245 (8)	0.0157 (8)	0.0201 (8)	0.0020 (6)	0.0063 (6)	0.0071 (6)
C12A	0.0228 (8)	0.0140 (7)	0.0201 (8)	0.0009 (6)	0.0046 (6)	0.0033 (6)
C13A	0.0233 (8)	0.0194 (8)	0.0254 (9)	−0.0003 (7)	0.0070 (7)	0.0066 (7)
C14A	0.0221 (9)	0.0234 (9)	0.0308 (10)	0.0001 (7)	0.0045 (7)	0.0039 (8)
C15A	0.0282 (9)	0.0177 (8)	0.0265 (9)	0.0019 (7)	0.0004 (7)	0.0025 (7)
C16A	0.0310 (9)	0.0211 (9)	0.0215 (8)	0.0015 (7)	0.0023 (7)	0.0069 (7)
C17A	0.0258 (9)	0.0188 (8)	0.0205 (8)	0.0008 (7)	0.0054 (6)	0.0058 (6)
C18A	0.0366 (12)	0.0344 (12)	0.0342 (12)	0.0026 (10)	−0.0068 (9)	0.0055 (9)
C19A	0.0214 (8)	0.0185 (8)	0.0313 (10)	0.0009 (7)	0.0088 (7)	0.0035 (7)
C20A	0.0353 (10)	0.0237 (9)	0.0193 (8)	0.0007 (8)	0.0052 (7)	0.0084 (7)
C21A	0.0350 (10)	0.0173 (8)	0.0199 (8)	−0.0002 (7)	0.0049 (7)	0.0047 (6)
C22A	0.0323 (10)	0.0264 (10)	0.0274 (10)	−0.0040 (8)	−0.0024 (8)	0.0087 (8)

Cl1B	0.0447 (3)	0.0339 (3)	0.0246 (2)	0.0120 (2)	0.0030 (2)	0.0165 (2)
S1B	0.01894 (19)	0.01488 (19)	0.01896 (19)	0.00212 (14)	0.00337 (14)	0.00674 (15)
O1B	0.0193 (6)	0.0195 (6)	0.0274 (7)	0.0047 (5)	0.0041 (5)	0.0110 (5)
O2B	0.0249 (6)	0.0204 (6)	0.0182 (6)	0.0019 (5)	0.0052 (5)	0.0073 (5)
N1B	0.0238 (7)	0.0137 (6)	0.0191 (7)	0.0022 (5)	0.0055 (5)	0.0053 (5)
N2B	0.0235 (7)	0.0154 (7)	0.0163 (6)	0.0068 (5)	0.0039 (5)	0.0050 (5)
C1B	0.0232 (8)	0.0165 (8)	0.0204 (8)	0.0044 (6)	0.0064 (6)	0.0073 (6)
C2B	0.0170 (7)	0.0141 (7)	0.0195 (7)	0.0021 (6)	0.0046 (6)	0.0061 (6)
C3B	0.0170 (7)	0.0196 (8)	0.0179 (7)	0.0026 (6)	0.0038 (6)	0.0063 (6)
C4B	0.0179 (7)	0.0169 (8)	0.0190 (7)	0.0017 (6)	0.0037 (6)	0.0059 (6)
C5B	0.0232 (8)	0.0240 (9)	0.0198 (8)	0.0034 (7)	0.0042 (6)	0.0100 (7)
C6B	0.0251 (8)	0.0211 (8)	0.0210 (8)	0.0020 (7)	0.0013 (6)	0.0096 (7)
C7B	0.0224 (8)	0.0182 (8)	0.0255 (9)	0.0017 (6)	0.0036 (6)	0.0092 (7)
C8B	0.0222 (8)	0.0174 (8)	0.0200 (8)	0.0029 (6)	0.0025 (6)	0.0062 (6)
C9B	0.0159 (7)	0.0170 (8)	0.0182 (7)	0.0003 (6)	0.0024 (5)	0.0064 (6)
C10B	0.0190 (7)	0.0144 (7)	0.0193 (7)	0.0020 (6)	0.0033 (6)	0.0060 (6)
C11B	0.0215 (8)	0.0139 (7)	0.0193 (7)	0.0028 (6)	0.0053 (6)	0.0044 (6)
C12B	0.0212 (8)	0.0158 (8)	0.0194 (8)	0.0022 (6)	0.0033 (6)	0.0059 (6)
C13B	0.0217 (8)	0.0213 (9)	0.0220 (8)	0.0042 (7)	0.0061 (6)	0.0078 (7)
C14B	0.0194 (8)	0.0246 (9)	0.0232 (8)	0.0018 (7)	0.0025 (6)	0.0069 (7)
C15B	0.0263 (9)	0.0254 (10)	0.0222 (9)	0.0004 (7)	0.0008 (7)	0.0053 (7)
C16B	0.0291 (9)	0.0257 (10)	0.0217 (9)	0.0043 (8)	0.0001 (7)	−0.0009 (7)
C17B	0.0237 (9)	0.0222 (9)	0.0238 (9)	0.0053 (7)	0.0040 (7)	0.0037 (7)
C18B	0.0291 (10)	0.0367 (12)	0.0329 (11)	−0.0006 (9)	−0.0039 (8)	0.0000 (9)
C19B	0.0221 (8)	0.0232 (9)	0.0262 (9)	0.0019 (7)	0.0088 (7)	0.0113 (7)
C20B	0.0271 (9)	0.0202 (9)	0.0206 (8)	0.0038 (7)	0.0039 (7)	0.0032 (7)
C21B	0.0266 (8)	0.0163 (8)	0.0175 (7)	0.0040 (6)	0.0031 (6)	0.0048 (6)
C22B	0.0236 (8)	0.0206 (9)	0.0249 (9)	0.0023 (7)	0.0000 (7)	0.0052 (7)

Geometric parameters (Å, °)

Cl1A—C6A	1.7461 (18)	Cl1B—C6B	1.7464 (19)
S1A—O2A	1.4348 (13)	S1B—O2B	1.4342 (13)
S1A—O1A	1.4386 (13)	S1B—O1B	1.4400 (13)
S1A—N1A	1.6158 (16)	S1B—N1B	1.6168 (15)
S1A—C12A	1.7678 (19)	S1B—C12B	1.7639 (18)
N1A—C1A	1.488 (2)	N1B—C1B	1.492 (2)
N1A—C11A	1.497 (2)	N1B—C11B	1.504 (2)
N2A—C9A	1.407 (2)	N2B—C9B	1.393 (2)
N2A—C10A	1.453 (2)	N2B—C10B	1.440 (2)
N2A—H1N	0.86 (2)	N2B—H2N	0.92 (2)
C1A—C2A	1.521 (2)	C1B—C2B	1.529 (2)
C1A—H1A	0.97	C1B—H1C	0.97
C1A—H1B	0.97	C1B—H1D	0.97
C2A—C10A	1.520 (2)	C2B—C10B	1.515 (2)
C2A—C3A	1.534 (2)	C2B—C3B	1.535 (2)
C2A—H2A	0.98	C2B—H2B	0.98
C3A—C20A	1.534 (3)	C3B—C19B	1.538 (2)
C3A—C19A	1.537 (2)	C3B—C20B	1.540 (3)

C3A—C4A	1.540 (2)	C3B—C4B	1.541 (2)
C4A—C5A	1.404 (2)	C4B—C5B	1.393 (2)
C4A—C9A	1.406 (2)	C4B—C9B	1.418 (2)
C5A—C6A	1.384 (3)	C5B—C6B	1.384 (3)
C5A—H5A	0.93	C5B—H5B	0.93
C6A—C7A	1.381 (3)	C6B—C7B	1.380 (3)
C7A—C8A	1.391 (3)	C7B—C8B	1.384 (3)
C7A—H7A	0.93	C7B—H7B	0.93
C8A—C9A	1.407 (2)	C8B—C9B	1.399 (2)
C8A—H8A	0.93	C8B—H8B	0.93
C10A—C11A	1.530 (2)	C10B—C11B	1.531 (2)
C10A—H10A	0.98	C10B—H10B	0.98
C11A—C21A	1.527 (3)	C11B—C21B	1.526 (2)
C11A—H11A	0.98	C11B—H11B	0.98
C12A—C13A	1.390 (2)	C12B—C13B	1.394 (2)
C12A—C17A	1.394 (3)	C12B—C17B	1.396 (3)
C13A—C14A	1.385 (3)	C13B—C14B	1.383 (3)
C13A—H13A	0.93	C13B—H13B	0.93
C14A—C15A	1.400 (3)	C14B—C15B	1.397 (3)
C14A—H14A	0.93	C14B—H14B	0.93
C15A—C16A	1.392 (3)	C15B—C16B	1.391 (3)
C15A—C18A	1.498 (3)	C15B—C18B	1.502 (3)
C16A—C17A	1.393 (3)	C16B—C17B	1.391 (3)
C16A—H16A	0.93	C16B—H16B	0.93
C17A—H17A	0.93	C17B—H17B	0.93
C18A—H18A	0.96	C18B—H18D	0.96
C18A—H18B	0.96	C18B—H18E	0.96
C18A—H18C	0.96	C18B—H18F	0.96
C19A—H19A	0.96	C19B—H19D	0.96
C19A—H19B	0.96	C19B—H19E	0.96
C19A—H19C	0.96	C19B—H19F	0.96
C20A—H20A	0.96	C20B—H20D	0.96
C20A—H20B	0.96	C20B—H20E	0.96
C20A—H20C	0.96	C20B—H20F	0.96
C21A—C22A	1.519 (3)	C21B—C22B	1.524 (3)
C21A—H21A	0.97	C21B—H21C	0.97
C21A—H21B	0.97	C21B—H21D	0.97
C22A—H22A	0.96	C22B—H22D	0.96
C22A—H22B	0.96	C22B—H22E	0.96
C22A—H22C	0.96	C22B—H22F	0.96
O2A—S1A—O1A	118.70 (8)	O2B—S1B—O1B	118.68 (8)
O2A—S1A—N1A	107.12 (8)	O2B—S1B—N1B	107.05 (8)
O1A—S1A—N1A	107.64 (8)	O1B—S1B—N1B	107.61 (8)
O2A—S1A—C12A	107.94 (8)	O2B—S1B—C12B	108.35 (8)
O1A—S1A—C12A	106.25 (8)	O1B—S1B—C12B	106.72 (8)
N1A—S1A—C12A	108.91 (8)	N1B—S1B—C12B	108.05 (8)
C1A—N1A—C11A	112.06 (14)	C1B—N1B—C11B	111.10 (13)
C1A—N1A—S1A	119.43 (12)	C1B—N1B—S1B	118.30 (12)
C11A—N1A—S1A	121.91 (12)	C11B—N1B—S1B	120.47 (11)

C9A—N2A—C10A	114.60 (14)	C9B—N2B—C10B	115.59 (14)
C9A—N2A—H1N	109.4 (17)	C9B—N2B—H2N	112.5 (15)
C10A—N2A—H1N	112.3 (16)	C10B—N2B—H2N	117.8 (14)
N1A—C1A—C2A	102.13 (13)	N1B—C1B—C2B	101.93 (13)
N1A—C1A—H1A	111.3	N1B—C1B—H1C	111.4
C2A—C1A—H1A	111.3	C2B—C1B—H1C	111.4
N1A—C1A—H1B	111.3	N1B—C1B—H1D	111.4
C2A—C1A—H1B	111.3	C2B—C1B—H1D	111.4
H1A—C1A—H1B	109.2	H1C—C1B—H1D	109.2
C10A—C2A—C1A	101.59 (14)	C10B—C2B—C1B	100.76 (13)
C10A—C2A—C3A	112.53 (14)	C10B—C2B—C3B	113.27 (14)
C1A—C2A—C3A	119.02 (14)	C1B—C2B—C3B	119.50 (14)
C10A—C2A—H2A	107.7	C10B—C2B—H2B	107.5
C1A—C2A—H2A	107.7	C1B—C2B—H2B	107.5
C3A—C2A—H2A	107.7	C3B—C2B—H2B	107.5
C2A—C3A—C20A	108.39 (14)	C2B—C3B—C19B	112.11 (14)
C2A—C3A—C19A	112.48 (14)	C2B—C3B—C20B	108.52 (15)
C20A—C3A—C19A	109.06 (15)	C19B—C3B—C20B	108.39 (14)
C2A—C3A—C4A	107.19 (13)	C2B—C3B—C4B	107.25 (13)
C20A—C3A—C4A	111.20 (14)	C19B—C3B—C4B	108.95 (15)
C19A—C3A—C4A	108.53 (14)	C20B—C3B—C4B	111.65 (14)
C5A—C4A—C9A	118.23 (16)	C5B—C4B—C9B	117.77 (16)
C5A—C4A—C3A	119.12 (15)	C5B—C4B—C3B	119.96 (15)
C9A—C4A—C3A	122.65 (15)	C9B—C4B—C3B	122.27 (15)
C6A—C5A—C4A	121.10 (16)	C6B—C5B—C4B	121.21 (17)
C6A—C5A—H5A	119.5	C6B—C5B—H5B	119.4
C4A—C5A—H5A	119.5	C4B—C5B—H5B	119.4
C7A—C6A—C5A	121.01 (17)	C7B—C6B—C5B	121.31 (17)
C7A—C6A—Cl1A	120.07 (14)	C7B—C6B—Cl1B	118.74 (15)
C5A—C6A—Cl1A	118.93 (14)	C5B—C6B—Cl1B	119.95 (14)
C6A—C7A—C8A	118.97 (17)	C6B—C7B—C8B	118.53 (17)
C6A—C7A—H7A	120.5	C6B—C7B—H7B	120.7
C8A—C7A—H7A	120.5	C8B—C7B—H7B	120.7
C7A—C8A—C9A	120.96 (16)	C7B—C8B—C9B	121.40 (17)
C7A—C8A—H8A	119.5	C7B—C8B—H8B	119.3
C9A—C8A—H8A	119.5	C9B—C8B—H8B	119.3
C4A—C9A—N2A	122.15 (15)	N2B—C9B—C8B	118.31 (15)
C4A—C9A—C8A	119.71 (16)	N2B—C9B—C4B	121.95 (15)
N2A—C9A—C8A	118.09 (15)	C8B—C9B—C4B	119.67 (16)
N2A—C10A—C2A	108.91 (14)	N2B—C10B—C2B	109.82 (14)
N2A—C10A—C11A	114.18 (14)	N2B—C10B—C11B	113.66 (14)
C2A—C10A—C11A	104.83 (14)	C2B—C10B—C11B	104.28 (14)
N2A—C10A—H10A	109.6	N2B—C10B—H10B	109.6
C2A—C10A—H10A	109.6	C2B—C10B—H10B	109.6
C11A—C10A—H10A	109.6	C11B—C10B—H10B	109.6
N1A—C11A—C21A	112.18 (15)	N1B—C11B—C21B	112.12 (14)
N1A—C11A—C10A	100.94 (13)	N1B—C11B—C10B	101.06 (13)
C21A—C11A—C10A	114.74 (15)	C21B—C11B—C10B	115.60 (15)
N1A—C11A—H11A	109.5	N1B—C11B—H11B	109.2

C21A—C11A—H11A	109.5	C21B—C11B—H11B	109.2
C10A—C11A—H11A	109.5	C10B—C11B—H11B	109.2
C13A—C12A—C17A	120.83 (17)	C13B—C12B—C17B	120.51 (17)
C13A—C12A—S1A	119.23 (14)	C13B—C12B—S1B	119.56 (14)
C17A—C12A—S1A	119.83 (14)	C17B—C12B—S1B	119.91 (14)
C14A—C13A—C12A	119.41 (18)	C14B—C13B—C12B	119.41 (17)
C14A—C13A—H13A	120.3	C14B—C13B—H13B	120.3
C12A—C13A—H13A	120.3	C12B—C13B—H13B	120.3
C13A—C14A—C15A	121.12 (18)	C13B—C14B—C15B	121.10 (17)
C13A—C14A—H14A	119.4	C13B—C14B—H14B	119.5
C15A—C14A—H14A	119.4	C15B—C14B—H14B	119.5
C16A—C15A—C14A	118.36 (18)	C16B—C15B—C14B	118.70 (17)
C16A—C15A—C18A	121.0 (2)	C16B—C15B—C18B	120.82 (18)
C14A—C15A—C18A	120.66 (19)	C14B—C15B—C18B	120.48 (18)
C15A—C16A—C17A	121.46 (18)	C17B—C16B—C15B	121.18 (18)
C15A—C16A—H16A	119.3	C17B—C16B—H16B	119.4
C17A—C16A—H16A	119.3	C15B—C16B—H16B	119.4
C16A—C17A—C12A	118.80 (18)	C16B—C17B—C12B	119.05 (17)
C16A—C17A—H17A	120.6	C16B—C17B—H17B	120.5
C12A—C17A—H17A	120.6	C12B—C17B—H17B	120.5
C15A—C18A—H18A	109.5	C15B—C18B—H18D	109.5
C15A—C18A—H18B	109.5	C15B—C18B—H18E	109.5
H18A—C18A—H18B	109.5	H18D—C18B—H18E	109.5
C15A—C18A—H18C	109.5	C15B—C18B—H18F	109.5
H18A—C18A—H18C	109.5	H18D—C18B—H18F	109.5
H18B—C18A—H18C	109.5	H18E—C18B—H18F	109.5
C3A—C19A—H19A	109.5	C3B—C19B—H19D	109.5
C3A—C19A—H19B	109.5	C3B—C19B—H19E	109.5
H19A—C19A—H19B	109.5	H19D—C19B—H19E	109.5
C3A—C19A—H19C	109.5	C3B—C19B—H19F	109.5
H19A—C19A—H19C	109.5	H19D—C19B—H19F	109.5
H19B—C19A—H19C	109.5	H19E—C19B—H19F	109.5
C3A—C20A—H20A	109.5	C3B—C20B—H20D	109.5
C3A—C20A—H20B	109.5	C3B—C20B—H20E	109.5
H20A—C20A—H20B	109.5	H20D—C20B—H20E	109.5
C3A—C20A—H20C	109.5	C3B—C20B—H20F	109.5
H20A—C20A—H20C	109.5	H20D—C20B—H20F	109.5
H20B—C20A—H20C	109.5	H20E—C20B—H20F	109.5
C22A—C21A—C11A	114.05 (16)	C22B—C21B—C11B	114.96 (15)
C22A—C21A—H21A	108.7	C22B—C21B—H21C	108.5
C11A—C21A—H21A	108.7	C11B—C21B—H21C	108.5
C22A—C21A—H21B	108.7	C22B—C21B—H21D	108.5
C11A—C21A—H21B	108.7	C11B—C21B—H21D	108.5
H21A—C21A—H21B	107.6	H21C—C21B—H21D	107.5
C21A—C22A—H22A	109.5	C21B—C22B—H22D	109.5
C21A—C22A—H22B	109.5	C21B—C22B—H22E	109.5
H22A—C22A—H22B	109.5	H22D—C22B—H22E	109.5
C21A—C22A—H22C	109.5	C21B—C22B—H22F	109.5
H22A—C22A—H22C	109.5	H22D—C22B—H22F	109.5

H22B—C22A—H22C	109.5	H22E—C22B—H22F	109.5
O2A—S1A—N1A—C1A	169.39 (13)	O2B—S1B—N1B—C1B	−163.44 (12)
O1A—S1A—N1A—C1A	−61.91 (15)	O1B—S1B—N1B—C1B	67.95 (14)
C12A—S1A—N1A—C1A	52.88 (15)	C12B—S1B—N1B—C1B	−46.94 (14)
O2A—S1A—N1A—C11A	20.15 (17)	O2B—S1B—N1B—C11B	−21.14 (15)
O1A—S1A—N1A—C11A	148.85 (14)	O1B—S1B—N1B—C11B	−149.75 (13)
C12A—S1A—N1A—C11A	−96.36 (15)	C12B—S1B—N1B—C11B	95.36 (14)
C11A—N1A—C1A—C2A	18.75 (19)	C11B—N1B—C1B—C2B	−20.22 (17)
S1A—N1A—C1A—C2A	−133.32 (13)	S1B—N1B—C1B—C2B	125.39 (13)
N1A—C1A—C2A—C10A	−37.04 (17)	N1B—C1B—C2B—C10B	39.55 (16)
N1A—C1A—C2A—C3A	−161.17 (15)	N1B—C1B—C2B—C3B	164.26 (14)
C10A—C2A—C3A—C20A	165.99 (15)	C10B—C2B—C3B—C19B	74.60 (18)
C1A—C2A—C3A—C20A	−75.4 (2)	C1B—C2B—C3B—C19B	−43.9 (2)
C10A—C2A—C3A—C19A	−73.34 (18)	C10B—C2B—C3B—C20B	−165.71 (14)
C1A—C2A—C3A—C19A	45.3 (2)	C1B—C2B—C3B—C20B	75.82 (19)
C10A—C2A—C3A—C4A	45.87 (18)	C10B—C2B—C3B—C4B	−44.95 (18)
C1A—C2A—C3A—C4A	164.48 (15)	C1B—C2B—C3B—C4B	−163.41 (15)
C2A—C3A—C4A—C5A	164.43 (15)	C2B—C3B—C4B—C5B	−162.76 (16)
C20A—C3A—C4A—C5A	46.1 (2)	C19B—C3B—C4B—C5B	75.7 (2)
C19A—C3A—C4A—C5A	−73.84 (19)	C20B—C3B—C4B—C5B	−44.0 (2)
C2A—C3A—C4A—C9A	−16.6 (2)	C2B—C3B—C4B—C9B	18.1 (2)
C20A—C3A—C4A—C9A	−134.87 (17)	C19B—C3B—C4B—C9B	−103.45 (18)
C19A—C3A—C4A—C9A	105.17 (18)	C20B—C3B—C4B—C9B	136.87 (17)
C9A—C4A—C5A—C6A	0.3 (2)	C9B—C4B—C5B—C6B	1.0 (3)
C3A—C4A—C5A—C6A	179.31 (16)	C3B—C4B—C5B—C6B	−178.19 (17)
C4A—C5A—C6A—C7A	−1.4 (3)	C4B—C5B—C6B—C7B	1.8 (3)
C4A—C5A—C6A—Cl1A	178.35 (13)	C4B—C5B—C6B—Cl1B	−177.53 (14)
C5A—C6A—C7A—C8A	0.9 (3)	C5B—C6B—C7B—C8B	−2.0 (3)
Cl1A—C6A—C7A—C8A	−178.84 (14)	Cl1B—C6B—C7B—C8B	177.33 (14)
C6A—C7A—C8A—C9A	0.7 (3)	C6B—C7B—C8B—C9B	−0.6 (3)
C5A—C4A—C9A—N2A	−176.24 (15)	C10B—N2B—C9B—C8B	−159.63 (16)
C3A—C4A—C9A—N2A	4.8 (2)	C10B—N2B—C9B—C4B	23.4 (2)
C5A—C4A—C9A—C8A	1.3 (2)	C7B—C8B—C9B—N2B	−173.72 (16)
C3A—C4A—C9A—C8A	−177.75 (15)	C7B—C8B—C9B—C4B	3.3 (3)
C10A—N2A—C9A—C4A	−22.4 (2)	C5B—C4B—C9B—N2B	173.47 (16)
C10A—N2A—C9A—C8A	160.05 (15)	C3B—C4B—C9B—N2B	−7.4 (2)
C7A—C8A—C9A—C4A	−1.8 (3)	C5B—C4B—C9B—C8B	−3.5 (2)
C7A—C8A—C9A—N2A	175.84 (16)	C3B—C4B—C9B—C8B	175.69 (16)
C9A—N2A—C10A—C2A	50.99 (19)	C9B—N2B—C10B—C2B	−49.7 (2)
C9A—N2A—C10A—C11A	167.75 (15)	C9B—N2B—C10B—C11B	−166.04 (14)
C1A—C2A—C10A—N2A	166.05 (14)	C1B—C2B—C10B—N2B	−168.06 (14)
C3A—C2A—C10A—N2A	−65.55 (18)	C3B—C2B—C10B—N2B	63.10 (18)
C1A—C2A—C10A—C11A	43.47 (17)	C1B—C2B—C10B—C11B	−45.92 (16)
C3A—C2A—C10A—C11A	171.87 (14)	C3B—C2B—C10B—C11B	−174.77 (13)
C1A—N1A—C11A—C21A	130.09 (16)	C1B—N1B—C11B—C21B	−131.15 (15)
S1A—N1A—C11A—C21A	−78.63 (19)	S1B—N1B—C11B—C21B	84.10 (17)
C1A—N1A—C11A—C10A	7.46 (18)	C1B—N1B—C11B—C10B	−7.46 (17)
S1A—N1A—C11A—C10A	158.74 (13)	S1B—N1B—C11B—C10B	−152.21 (12)
N2A—C10A—C11A—N1A	−150.26 (14)	N2B—C10B—C11B—N1B	152.44 (14)

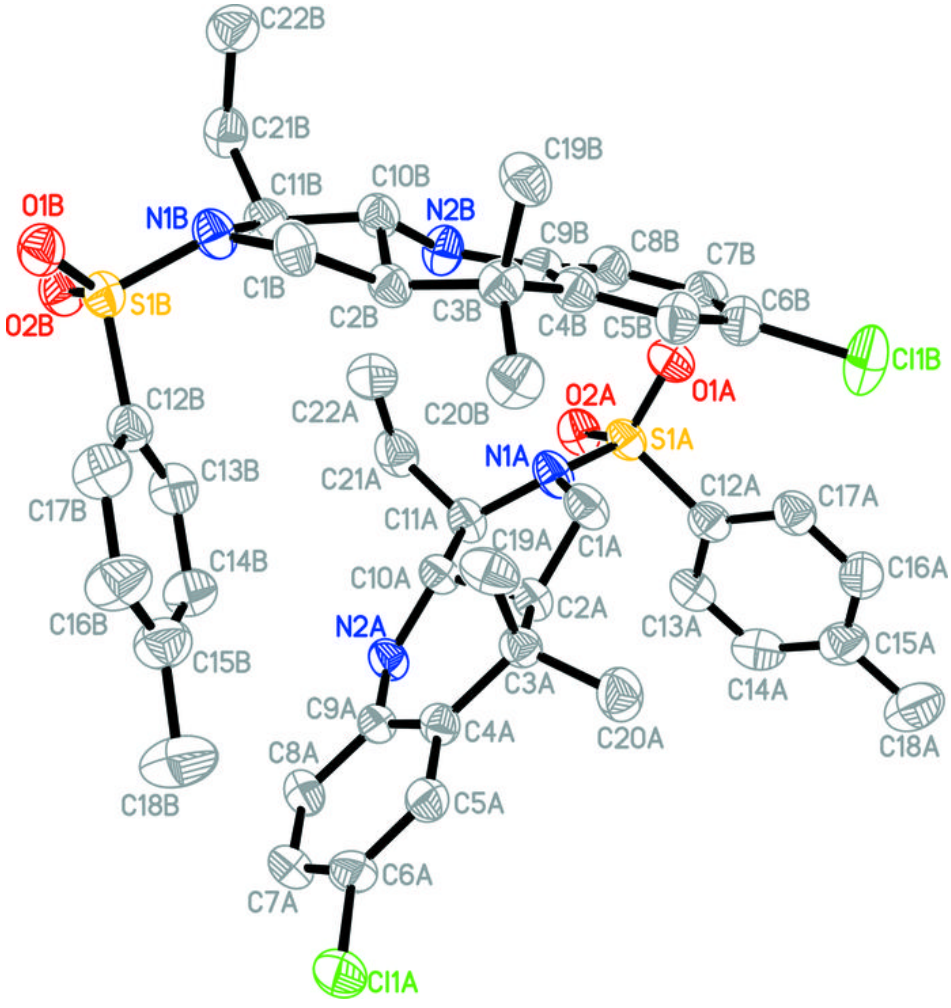
C2A—C10A—C11A—N1A	−31.16 (17)	C2B—C10B—C11B—N1B	32.87 (16)
N2A—C10A—C11A—C21A	88.91 (19)	N2B—C10B—C11B—C21B	−86.29 (19)
C2A—C10A—C11A—C21A	−151.99 (15)	C2B—C10B—C11B—C21B	154.14 (14)
O2A—S1A—C12A—C13A	−31.57 (17)	O2B—S1B—C12B—C13B	42.10 (17)
O1A—S1A—C12A—C13A	−159.90 (14)	O1B—S1B—C12B—C13B	170.97 (14)
N1A—S1A—C12A—C13A	84.40 (16)	N1B—S1B—C12B—C13B	−73.55 (16)
O2A—S1A—C12A—C17A	144.65 (14)	O2B—S1B—C12B—C17B	−136.14 (15)
O1A—S1A—C12A—C17A	16.32 (17)	O1B—S1B—C12B—C17B	−7.27 (18)
N1A—S1A—C12A—C17A	−99.38 (15)	N1B—S1B—C12B—C17B	108.20 (16)
C17A—C12A—C13A—C14A	−0.4 (3)	C17B—C12B—C13B—C14B	0.6 (3)
S1A—C12A—C13A—C14A	175.81 (14)	S1B—C12B—C13B—C14B	−177.67 (14)
C12A—C13A—C14A—C15A	−0.7 (3)	C12B—C13B—C14B—C15B	1.3 (3)
C13A—C14A—C15A—C16A	1.4 (3)	C13B—C14B—C15B—C16B	−1.8 (3)
C13A—C14A—C15A—C18A	−178.63 (19)	C13B—C14B—C15B—C18B	178.0 (2)
C14A—C15A—C16A—C17A	−1.1 (3)	C14B—C15B—C16B—C17B	0.4 (3)
C18A—C15A—C16A—C17A	178.96 (18)	C18B—C15B—C16B—C17B	−179.3 (2)
C15A—C16A—C17A—C12A	0.0 (3)	C15B—C16B—C17B—C12B	1.3 (3)
C13A—C12A—C17A—C16A	0.7 (3)	C13B—C12B—C17B—C16B	−1.9 (3)
S1A—C12A—C17A—C16A	−175.47 (14)	S1B—C12B—C17B—C16B	176.38 (16)
N1A—C11A—C21A—C22A	−54.6 (2)	N1B—C11B—C21B—C22B	56.5 (2)
C10A—C11A—C21A—C22A	59.8 (2)	C10B—C11B—C21B—C22B	−58.6 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2A—H1N···O1B^{i}	0.86 (3)	2.44 (2)	3.285 (2)	167 (2)
N2B—H2N···O1A^{ii}	0.92 (3)	2.29 (2)	3.188 (2)	165 (2)
C8A—H8A···O1B^{iii}	0.93	2.49	3.327 (2)	149
C21A—H21B···O1B^{i}	0.97	2.52	3.447 (3)	159
C1A—H1A···Cg1	0.97	2.92	3.760 (2)	145
C14A—H14A···Cg1^{iii}	0.93	3.00	3.876 (2)	158
C22B—H22D···Cg2^{ii}	0.97	2.84	3.558 (2)	133
C13A—H13A···O2A^{iv}	0.93	2.52	3.294 (2)	141
C21A—H21A···O2A	0.97	2.50	3.101 (3)	120
C21B—H21D···O2B	0.97	2.57	3.158 (1)	119

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

Fig. 1


C22B
C21B
C19B
C11B
C10B
O1B
N1B
N2B
C9B
C8B
C7B
C6B
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O2B
C1B
C2B
C3B
C4B
C5B
Cl1B
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O1A
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C21A
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C17A
C17B
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C14B
C10A
C16A
C2A
C16B
N2A
C13A
C15A
C15B
C3A
C14A
C9A
C4A
C20A
C18A
C8A
C18B
C5A
C6A
C7A
Cl1A

Fig. 2

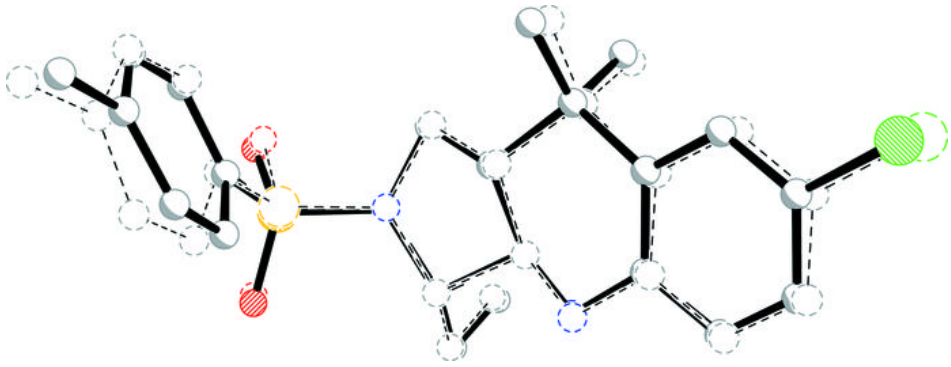

Fig. 3