Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Tetrabutylammonium 5-(2-hydroxyphenyl)-1,3,4-oxadiazole-2-thiolate

N. K. Singh,[a]* A. K. Pandey,[a] M. Singh,[a] M. K. Bharty[a] and Ray J. Butcher[b]

[a]Department of Chemistry, Banaras Hindu University, Varanasi 221 005, India, and [b]Department of Chemistry, Howard University, 525 College Street NW, Washington, DC 20059, USA
Correspondence e-mail: singhnk_bhu@yahoo.com

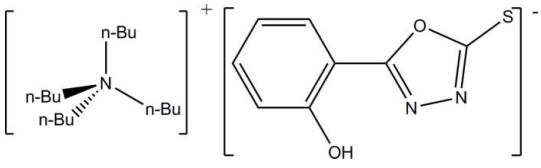
Received 30 September 2007; accepted 9 October 2007

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.004 Å; disorder in solvent or counterion; R factor = 0.050; wR factor = 0.150; data-to-parameter ratio = 22.0.

The title compound, $C_{16}H_{36}N^+\cdot C_8H_5N_2O_2S^-$, crystallizes with two formula units in the asymmetric unit. In both anions, the oxadiazole ring is almost coplanar with the 2-hydroxyphenyl ring. The anion structure is influenced by intramolecular O—H···N hydrogen bonding. The crystal packing is stabilized by intermolecular C—H···S, C—H···O, C—H···N and C—H···π interactions. One butyl group is disordered over two positions, with site-occupancy factors of *ca* 0.6 and 0.4.

Related literature

For related structures, see: Du & Zhao (2004); Singh *et al.* (2006); Singh *et al.* (2007); Stockhouse *et al.* (2001); Zhang *et al.* (2002).



Experimental

Crystal data

$C_{16}H_{36}N^+\cdot C_8H_5N_2O_2S^-$
M_r = 435.66
Monoclinic, $P2_1/n$
a = 16.600 (6) Å
b = 13.228 (5) Å
c = 23.957 (9) Å
β = 97.710 (6)°
V = 5213 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.15 mm^{-1}
T = 173 (2) K
0.51 × 0.43 × 0.23 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.929, T_{max} = 0.967
51583 measured reflections
12911 independent reflections
5952 reflections with $I > 2\sigma(I)$
R_{int} = 0.081

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.150
S = 0.99
12911 reflections
586 parameters
16 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

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

*Cg*1 is the centroid of the O1*A*/C1*A*/N1*A*/N2*A*/C2*A* ring and *Cg*2 is the centroid of the O1*B*/C1*B*/N1*B*/N2*B*/C2*B* ring.

D—H···A	D—H	H···A	D···A	D—H···A
O2*A*—H2*A*···N2*A*	0.90 (3)	1.86 (3)	2.665 (3)	148 (3)
O2*B*—H2*B*···N2*B*	0.87 (3)	1.90 (3)	2.645 (3)	143 (3)
C11*B*—H11*C*···N1*B*^{i}	0.99	2.47	3.440 (16)	165
C21*A*—H21*A*···N1*B*^{i}	0.99	2.57	3.551 (3)	172
C31*B*—H31*D*···O2*B*	0.99	2.58	3.511 (3)	157
C41*A*—H41*B*···S1*B*^{ii}	0.99	2.79	3.520 (3)	131
C11*C*—H11*E*···N1*B*^{i}	0.99	2.42	3.38 (3)	163
C41*B*—H41*C*···N1*A*	0.99	2.52	3.459 (3)	157
C24*B*—H24*E*···*Cg*1	0.99	2.92	3.863 (3)	159
C42*A*—H42*B*···*Cg*2^{iii}	0.99	2.93	3.576 (3)	125

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x+\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$; (iii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2006); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

RJB acknowledges the Naval Research Laboratory for access to their diffractometers.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2477).

References

Bruker (2000). *SHELXTL*. Version 6.12. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2004). *SADABS*. Version 2004/1. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2005). *SAINT*. Version 7.34a. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2006). *APEX2*. Version 2.1-0. Bruker AXS Inc., Madison, Wisconsin, USA.
Du, M. & Zhao, X.-J. (2004). *Acta Cryst.* C**60**, o54–o56.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1997). *SHELXL97*. Release 97-1. University of Göttingen, Germany.
Singh, N. K., Butcher, R. J., Bharty, M. K., Srivastava, A. K. & Tripathi, P. (2006). *Acta Cryst.* E**62**, o3473–o3474.
Singh, N. K., Butcher, R. J., Tripathi, P., Srivastava, A. K. & Bharty, M. K. (2007). *Acta Cryst.* E**63**, o782–o784.
Stockhouse, S., Wicklender, M. S., Meyer, G., Oryzall, I. & Schulz, B. (2001). *J. Mol. Struct.* **561**, 175–183.
Zhang, Y., Qiao, R. Z., Xu, P. F., Zhang, Z. Y., Wang, Q., Mao, L. M. & Yu, K. B. (2002). *J. Chin. Chem. Soc. (Taipei)*, **49**, 369–372.

 doi:10.1107/S1600536807049471

supplementary materials

Acta Cryst. (2007). E**63**, o4327 [**doi:10.1107/S1600536807049471**]

Tetrabutylammonium 5-(2-hydroxyphenyl)-1,3,4-oxadiazole-2-thiolate

N. K. Singh, A. K. Pandey, M. Singh, M. K. Bharty and R. J. Butcher

Comment

The title compound was synthesized by the ring closure reaction of the product obtained by the reaction of carbon disulfide with salicylic acid hydrazide in the presence of a base, followed by the addition of tetrabutylammoniumbromide in ethanolic medium.

The compound crystallizes in the monoclinic space group $P2_1/n$ with two formula units in the asymmetric unit. The contents of the asymmetric unit, together with the atom-labelling scheme, are shown in Fig 1. The bond lengths and angles of the 1,3,4-oxadiazole ring are in good agreement with the values quoted in previous reports (Zhang *et al.*, 2002; Singh *et al.* 2006, 2007; Stockhouse *et al.* 2001; Du & Zhao, 2004). The C1A—N1A [1.312 (3) Å] and C1B—N1B [1.308 (3) Å] bond lengths are intermediate between 1.47 Å for a C—N single bond and 1.29 Å for a C═N double bond, and are significantly longer than the C2A—N2A [1.287 (3) Å] and C2B—N2B [1.290 (3) Å] bond lengths. The C—S bond distances [S1A—C1A = 1.674 (3) Å and S1B—C1B [1.684 (2) Å] are also intermediate between 1.82 Å for a C—S single bond and 1.56 Å for a C═S double bond.

In both molecules, the oxadiazole ring is almost coplanar with the 2-hydroxyphenyl ring. The dihedral angle between the two rings is 6.6 (1)° for molecule A and 1.4 (1)° for molecule B.

The molecular structure of each independent anion is influenced by O2A–H2A···N2A or O2B–H2B···N2B intramolecular hydrogen bonding. In the crystal structure, weak intermolecular C—H···S, C—H···N, and C—H···O interactions are observed (Table 1). In addition, the crystal packing is reinforced by weak intermolecular C—H···π interactions involving the C42A—H42B bond and the O1B/C1B/N1B/N2B/C2B ring [H···ring centroid = 2.92 Å, C21B···ring centroid = 3.578 (3) Å]. Thus the planarity of the two rings, π-electron delocalization, intermolecular and intramolecular interactions all contribute to stabilize the structure of the compound.

Experimental

Compound (I) was synthesized by adding CS_2 (2.4 ml, 40 mmol) to a solution of salicylic acid hydrazide (3.04 g, 20 mmol) in ethanol (15 ml) in the presence of KOH (1.12 g, 20 mmol) and stirring the reaction mixture for 2 h at room temperature. The solid product obtained in the above reaction was dissolved in EtOH-H_2O mixture (75:25 *v*/*v*) and an EtOH solution of tetrabutylammonium bromide (3.22 g, 10 mmol) was added. The resulting dirty yellow solution was concentrated at room temperature to obtain solid of compound (I). The solid product was dissolved in minimum amount of ethanol (20 ml), to which water was added drop wise whereupon the impurity settled out. The solution was decanted and after evaporation of the solvent compound (I) solidified. White single crystals of (I) (m.p. 347 K) suitable for X-ray analysis were obtained by slow evaporation of a methanol solution over a period of 5 d. (yield 2.90 g, 68.75%): Analysis calculated: C 66.16, H 9.48, N 9.64%; found for $C_{24}H_{41}N_3O_2S$ (435.66): C 66.10, H 9.43, N 9.68%; IR (KBr, ν cm^{-1}): 3441 (OH), 1288 (C—O), 1601 (C=N), 1070 (N—N), 902 (C—S); ^{13}C NMR ($CDCl_3$, TMS): 179.78 (C1A), 160.81 (C2A), 124.71 (C3A), 160.25 (C4A),

133.35 (C5A), 129.33 (C6A), 118.10 (C7A), 128.91 (C8A), 57.52 (C11A, C21A, C31A, C41A), 23.04 (C12A, C22A, C32A, C32B, C42A), 19.16 (C13A, C23A, C33A, C43A), 13.42 (C14A, C24A, C34A, C44A).

Refinement

All H atoms were initially located in a difference Fourier map. C-bound H atoms were then constrained to an ideal geometry with C—H distances in the range of 0.95–0.99 Å and U_{iso}(H) = 1.2U_{eq}(C). O-bound H atoms were refined freely. One of the *n*-butyl arms of one of the two tetrabutylammonium cations is disordered over two conformations with occupancies of 0.641 (7) and 0.359 (7). Both conformers were constrained to have similar geometries.

Figures

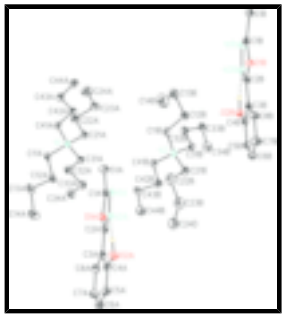


Fig. 1. The asymmetric unit of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 20% probability level. All H atoms, except H2A and H2B, are omitted for clarity.

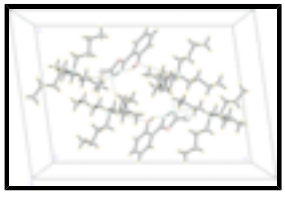


Fig. 2. The unit-cell contents of the title compound, showing intramolecular and intermolecular interactions as dashed lines.

Tetrabutylammonium 5-(2-hydroxyphenyl)-1,3,4-oxadiazole-2-thiolate

Crystal data

$C_{16}H_{36}N^{+}\cdot C_8H_5N_2O_2S^{-}$	F_{000} = 1904
M_r = 435.66	D_x = 1.110 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 7605 reflections
a = 16.600 (6) Å	θ = 2.2–24.2°
b = 13.228 (5) Å	μ = 0.15 mm^{-1}
c = 23.957 (9) Å	T = 173 (2) K
β = 97.710 (6)°	Plate, colorless
V = 5213 (3) Å^3	0.51 × 0.43 × 0.23 mm
Z = 8	

Data collection

Bruker APEXII CCD area-detector	12911 independent reflections

diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

T = 173(2) K

φ and ω scans

Absorption correction: multi-scan (SADABS; Bruker, 2004)

T_{min} = 0.929, T_{max} = 0.967

51583 measured reflections

5952 reflections with $I > 2\sigma(I)$

R_{int} = 0.081

θ_{max} = 28.4º

θ_{min} = 1.4º

$h = -21 \rightarrow 22$

$k = -17 \rightarrow 17$

$l = -32 \rightarrow 29$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.050

$wR(F^2)$ = 0.150

S = 0.99

12911 reflections

586 parameters

16 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0458P)^2 + 2.3996P]$ where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max}$ = 0.22 e Å^{-3}

$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Extinction correction: none

Special details

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}	Occ. (<1)
S1A	0.37223 (4)	0.70771 (5)	0.20112 (3)	0.0557 (2)	
O1A	0.30749 (9)	0.60789 (11)	0.10893 (6)	0.0412 (4)	
O2A	0.31975 (14)	0.31664 (15)	0.04194 (10)	0.0702 (6)	
H2A	0.3507 (19)	0.347 (2)	0.0708 (13)	0.079 (11)*	
N1A	0.39980 (12)	0.51807 (15)	0.16416 (9)	0.0465 (5)	
N2A	0.36975 (13)	0.46067 (15)	0.11638 (9)	0.0471 (5)	
C1A	0.36270 (14)	0.60585 (19)	0.15926 (10)	0.0416 (6)	

C2A	0.31688 (15)	0.51541 (18)	0.08591 (10)	0.0404 (6)
C3A	0.26839 (15)	0.48733 (19)	0.03352 (10)	0.0438 (6)
C4A	0.27140 (17)	0.3875 (2)	0.01407 (12)	0.0529 (7)
C5A	0.22353 (19)	0.3599 (2)	−0.03591 (13)	0.0657 (8)
H5A	0.2256	0.2926	−0.0496	0.079*
C6A	0.17315 (18)	0.4302 (3)	−0.06550 (13)	0.0691 (9)
H6A	0.1405	0.4108	−0.0994	0.083*
C7A	0.16958 (18)	0.5278 (3)	−0.04651 (12)	0.0664 (9)
H7A	0.1346	0.5754	−0.0672	0.080*
C8A	0.21686 (16)	0.5564 (2)	0.00271 (11)	0.0542 (7)
H8A	0.2143	0.6240	0.0158	0.065*
S1B	0.34712 (4)	0.71102 (5)	0.67823 (3)	0.04552 (17)
O1B	0.27317 (9)	0.60672 (11)	0.59033 (6)	0.0396 (4)
O2B	0.31007 (11)	0.33542 (13)	0.50700 (8)	0.0498 (5)
H2B	0.3400 (18)	0.360 (2)	0.5362 (12)	0.071 (10)*
N1B	0.38606 (12)	0.53313 (14)	0.63132 (9)	0.0424 (5)
N2B	0.35079 (12)	0.47286 (14)	0.58594 (8)	0.0416 (5)
C1B	0.33942 (14)	0.61234 (17)	0.63338 (10)	0.0374 (5)
C2B	0.28563 (14)	0.51866 (17)	0.56379 (10)	0.0370 (5)
C3B	0.22823 (15)	0.48426 (17)	0.51656 (10)	0.0390 (6)
C4B	0.24315 (15)	0.39264 (18)	0.49015 (10)	0.0416 (6)
C5B	0.18907 (16)	0.3588 (2)	0.44487 (11)	0.0496 (7)
H5B	0.1994	0.2972	0.4267	0.060*
C6B	0.12055 (18)	0.4140 (2)	0.42610 (12)	0.0571 (7)
H6B	0.0838	0.3901	0.3951	0.069*
C7B	0.10472 (19)	0.5043 (2)	0.45203 (12)	0.0642 (8)
H7B	0.0570	0.5417	0.4392	0.077*
C8B	0.15880 (16)	0.5394 (2)	0.49666 (11)	0.0522 (7)
H8B	0.1485	0.6018	0.5140	0.063*
N1	0.64839 (11)	0.57678 (14)	0.20150 (8)	0.0375 (5)
C11A	0.63841 (15)	0.64087 (18)	0.14823 (10)	0.0413 (6)
H11A	0.6500	0.7121	0.1591	0.050*
H11B	0.6799	0.6194	0.1246	0.050*
C12A	0.55586 (16)	0.6366 (2)	0.11253 (11)	0.0500 (7)
H12A	0.5450	0.5668	0.0986	0.060*
H12B	0.5131	0.6552	0.1358	0.060*
C13A	0.55304 (18)	0.7082 (2)	0.06317 (11)	0.0634 (8)
H13A	0.6037	0.7010	0.0460	0.076*
H13B	0.5505	0.7785	0.0770	0.076*
C14A	0.4807 (2)	0.6891 (3)	0.01852 (13)	0.0829 (10)
H14A	0.4817	0.7374	−0.0124	0.124*
H14B	0.4303	0.6976	0.0351	0.124*
H14C	0.4835	0.6201	0.0041	0.124*
C21A	0.59405 (14)	0.61311 (17)	0.24331 (10)	0.0403 (6)
H21A	0.6053	0.5713	0.2777	0.048*
H21B	0.5369	0.6007	0.2271	0.048*
C22A	0.60217 (16)	0.72338 (19)	0.26044 (11)	0.0482 (6)
H22A	0.5795	0.7668	0.2285	0.058*
H22B	0.6603	0.7408	0.2706	0.058*

C23A	0.55669 (16)	0.7419 (2)	0.31053 (11)	0.0540 (7)	
H23A	0.5847	0.7058	0.3438	0.065*	
H23B	0.5011	0.7139	0.3022	0.065*	
C24A	0.5515 (2)	0.8540 (2)	0.32434 (14)	0.0763 (10)	
H24A	0.5218	0.8625	0.3567	0.114*	
H24B	0.5228	0.8898	0.2918	0.114*	
H24C	0.6064	0.8817	0.3334	0.114*	
C31A	0.62430 (14)	0.46778 (16)	0.18865 (10)	0.0396 (6)	
H31A	0.5664	0.4663	0.1721	0.047*	
H31B	0.6291	0.4300	0.2246	0.047*	
C32A	0.67344 (16)	0.41286 (18)	0.14902 (11)	0.0474 (6)	
H32A	0.6709	0.4507	0.1132	0.057*	
H32B	0.7311	0.4090	0.1661	0.057*	
C33A	0.64023 (18)	0.30731 (19)	0.13752 (12)	0.0574 (7)	
H33A	0.5832	0.3119	0.1193	0.069*	
H33B	0.6405	0.2712	0.1737	0.069*	
C34A	0.6894 (2)	0.2470 (2)	0.09976 (13)	0.0681 (9)	
H34A	0.6657	0.1794	0.0935	0.102*	
H34B	0.7457	0.2410	0.1179	0.102*	
H34C	0.6884	0.2817	0.0635	0.102*	
C41A	0.73787 (14)	0.58491 (17)	0.22524 (10)	0.0406 (6)	
H41A	0.7703	0.5604	0.1962	0.049*	
H41B	0.7510	0.6574	0.2317	0.049*	
C42A	0.76561 (14)	0.52838 (18)	0.27942 (10)	0.0436 (6)	
H42A	0.7463	0.4576	0.2760	0.052*	
H42B	0.7424	0.5605	0.3110	0.052*	
C43A	0.85770 (15)	0.5303 (2)	0.29096 (11)	0.0505 (7)	
H43A	0.8762	0.6015	0.2941	0.061*	
H43B	0.8801	0.4995	0.2587	0.061*	
C44A	0.89112 (17)	0.4743 (2)	0.34442 (12)	0.0611 (8)	
H44A	0.9506	0.4780	0.3498	0.092*	
H44B	0.8741	0.4034	0.3413	0.092*	
H44C	0.8702	0.5054	0.3767	0.092*	
N2	0.37404 (12)	0.39697 (14)	0.33340 (9)	0.0435 (5)	
C11B	0.4069 (10)	0.4927 (8)	0.3637 (6)	0.043 (2)	0.641 (7)
H11C	0.4665	0.4849	0.3727	0.051*	0.641 (7)
H11D	0.3972	0.5493	0.3366	0.051*	0.641 (7)
C12B	0.3747 (8)	0.5252 (6)	0.4176 (3)	0.052 (2)	0.641 (7)
H12C	0.3885	0.4726	0.4467	0.063*	0.641 (7)
H12D	0.3147	0.5300	0.4102	0.063*	0.641 (7)
C13B	0.4091 (5)	0.6269 (5)	0.4404 (3)	0.074 (2)	0.641 (7)
H13C	0.3982	0.6349	0.4798	0.089*	0.641 (7)
H13D	0.4688	0.6269	0.4406	0.089*	0.641 (7)
C14B	0.3731 (5)	0.7151 (5)	0.4062 (3)	0.107 (3)	0.641 (7)
H14D	0.3971	0.7781	0.4224	0.160*	0.641 (7)
H14E	0.3142	0.7165	0.4066	0.160*	0.641 (7)
H14F	0.3846	0.7083	0.3673	0.160*	0.641 (7)
C11C	0.410 (2)	0.4999 (15)	0.3510 (12)	0.050 (5)	0.359 (7)
H11E	0.4692	0.4931	0.3647	0.060*	0.359 (7)

H11F	0.4038	0.5470	0.3186	0.060*	0.359 (7)
C12C	0.3654 (13)	0.5394 (10)	0.3978 (5)	0.050 (3)	0.359 (7)
H12E	0.3743	0.4943	0.4310	0.060*	0.359 (7)
H12F	0.3063	0.5432	0.3847	0.060*	0.359 (7)
C13C	0.3997 (8)	0.6445 (8)	0.4127 (4)	0.059 (3)	0.359 (7)
H13E	0.4592	0.6394	0.4235	0.071*	0.359 (7)
H13F	0.3897	0.6884	0.3790	0.071*	0.359 (7)
C14C	0.3624 (6)	0.6929 (8)	0.4603 (4)	0.083 (4)	0.359 (7)
H14G	0.3865	0.7598	0.4683	0.124*	0.359 (7)
H14H	0.3730	0.6504	0.4940	0.124*	0.359 (7)
H14I	0.3036	0.6997	0.4495	0.124*	0.359 (7)
C21B	0.28409 (14)	0.40714 (19)	0.31129 (12)	0.0487 (7)	
H21C	0.2660	0.3443	0.2909	0.058*	
H21D	0.2535	0.4130	0.3439	0.058*	
C22B	0.26181 (17)	0.4962 (2)	0.27233 (14)	0.0681 (9)	
H22C	0.3034	0.5043	0.2466	0.082*	
H22D	0.2611	0.5588	0.2949	0.082*	
C23B	0.17851 (19)	0.4807 (3)	0.23776 (15)	0.0759 (10)	
H23C	0.1396	0.4579	0.2630	0.091*	
H23D	0.1588	0.5461	0.2211	0.091*	
C24D	0.1803 (2)	0.4042 (3)	0.19130 (15)	0.0870 (11)	
H24D	0.1256	0.3969	0.1704	0.130*	
H24E	0.1986	0.3388	0.2076	0.130*	
H24F	0.2178	0.4270	0.1656	0.130*	
C31B	0.38041 (15)	0.31129 (18)	0.37581 (11)	0.0438 (6)	
H31C	0.3556	0.2502	0.3568	0.053*	
H31D	0.3478	0.3293	0.4061	0.053*	
C32B	0.46590 (16)	0.2847 (2)	0.40281 (11)	0.0527 (7)	
H32C	0.4897	0.3429	0.4252	0.063*	
H32D	0.5003	0.2707	0.3730	0.063*	
C33B	0.46514 (18)	0.1922 (2)	0.44100 (12)	0.0591 (8)	
H33C	0.5200	0.1837	0.4625	0.071*	
H33D	0.4267	0.2047	0.4685	0.071*	
C34B	0.4413 (2)	0.0947 (2)	0.40990 (14)	0.0763 (10)	
H34D	0.4422	0.0391	0.4370	0.114*	
H34E	0.4799	0.0804	0.3833	0.114*	
H34F	0.3865	0.1015	0.3893	0.114*	
C41B	0.42319 (15)	0.37380 (18)	0.28570 (11)	0.0447 (6)	
H41C	0.4168	0.4309	0.2588	0.054*	
H41D	0.4813	0.3704	0.3016	0.054*	
C42B	0.40114 (17)	0.2770 (2)	0.25339 (12)	0.0578 (7)	
H42C	0.4079	0.2186	0.2795	0.069*	
H42D	0.3435	0.2796	0.2361	0.069*	
C43B	0.45533 (17)	0.2639 (2)	0.20792 (11)	0.0533 (7)	
H43C	0.4516	0.3254	0.1842	0.064*	
H43D	0.5124	0.2573	0.2259	0.064*	
C44B	0.4340 (2)	0.1731 (3)	0.17077 (14)	0.0787 (10)	
H44D	0.4712	0.1691	0.1424	0.118*	
H44E	0.3780	0.1797	0.1520	0.118*	

H44F	0.4388	0.1117	0.1938	0.118*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1A	0.0585 (4)	0.0526 (4)	0.0529 (4)	0.0059 (3)	−0.0040 (3)	−0.0101 (3)
O1A	0.0441 (10)	0.0398 (9)	0.0383 (9)	0.0044 (8)	0.0005 (8)	0.0001 (8)
O2A	0.0852 (16)	0.0477 (12)	0.0773 (16)	0.0024 (11)	0.0094 (13)	−0.0132 (11)
N1A	0.0467 (12)	0.0457 (12)	0.0459 (13)	0.0045 (10)	0.0019 (10)	0.0042 (10)
N2A	0.0516 (13)	0.0426 (12)	0.0471 (13)	0.0040 (10)	0.0067 (11)	0.0010 (10)
C1A	0.0400 (14)	0.0481 (15)	0.0365 (13)	0.0001 (11)	0.0041 (11)	0.0043 (11)
C2A	0.0426 (14)	0.0386 (13)	0.0414 (14)	−0.0001 (11)	0.0102 (12)	0.0004 (11)
C3A	0.0427 (14)	0.0504 (15)	0.0404 (14)	−0.0037 (12)	0.0129 (12)	−0.0027 (12)
C4A	0.0529 (17)	0.0539 (16)	0.0546 (17)	−0.0054 (14)	0.0169 (14)	−0.0099 (14)
C5A	0.065 (2)	0.073 (2)	0.062 (2)	−0.0159 (17)	0.0195 (17)	−0.0236 (17)
C6A	0.0542 (19)	0.106 (3)	0.0481 (18)	−0.0170 (19)	0.0126 (15)	−0.0217 (19)
C7A	0.0557 (18)	0.096 (2)	0.0457 (17)	0.0006 (17)	0.0012 (14)	−0.0049 (17)
C8A	0.0514 (16)	0.0648 (17)	0.0457 (16)	0.0025 (14)	0.0038 (13)	−0.0029 (14)
S1B	0.0513 (4)	0.0428 (3)	0.0421 (4)	0.0025 (3)	0.0049 (3)	−0.0048 (3)
O1B	0.0439 (9)	0.0357 (8)	0.0380 (9)	0.0056 (7)	0.0007 (8)	−0.0002 (7)
O2B	0.0505 (11)	0.0465 (10)	0.0533 (12)	0.0046 (9)	0.0100 (10)	−0.0082 (9)
N1B	0.0405 (11)	0.0397 (11)	0.0464 (12)	0.0028 (9)	0.0041 (10)	0.0003 (10)
N2B	0.0427 (12)	0.0388 (11)	0.0430 (12)	0.0038 (9)	0.0049 (10)	−0.0010 (9)
C1B	0.0381 (13)	0.0398 (13)	0.0346 (13)	−0.0010 (11)	0.0057 (11)	0.0039 (11)
C2B	0.0432 (14)	0.0340 (12)	0.0354 (13)	0.0015 (11)	0.0114 (11)	0.0001 (11)
C3B	0.0465 (14)	0.0371 (12)	0.0341 (13)	−0.0001 (11)	0.0076 (11)	0.0038 (11)
C4B	0.0482 (15)	0.0403 (13)	0.0385 (14)	−0.0020 (12)	0.0142 (12)	0.0033 (11)
C5B	0.0600 (17)	0.0452 (14)	0.0456 (15)	−0.0118 (13)	0.0139 (14)	−0.0070 (12)
C6B	0.0644 (19)	0.0609 (18)	0.0440 (16)	−0.0100 (15)	−0.0006 (14)	−0.0033 (14)
C7B	0.071 (2)	0.0609 (18)	0.0546 (18)	0.0086 (15)	−0.0146 (16)	0.0024 (15)
C8B	0.0615 (17)	0.0459 (15)	0.0462 (16)	0.0075 (13)	−0.0043 (14)	−0.0007 (12)
N1	0.0410 (11)	0.0337 (10)	0.0383 (11)	−0.0015 (9)	0.0069 (9)	0.0021 (9)
C11A	0.0478 (15)	0.0391 (13)	0.0385 (13)	−0.0009 (11)	0.0112 (12)	0.0073 (11)
C12A	0.0507 (16)	0.0569 (16)	0.0424 (15)	0.0006 (13)	0.0066 (13)	0.0110 (13)
C13A	0.0642 (19)	0.078 (2)	0.0485 (16)	0.0110 (16)	0.0103 (15)	0.0168 (16)
C14A	0.086 (2)	0.100 (3)	0.059 (2)	0.019 (2)	−0.0053 (18)	0.0095 (19)
C21A	0.0397 (13)	0.0449 (14)	0.0369 (13)	0.0021 (11)	0.0082 (11)	0.0023 (11)
C22A	0.0485 (15)	0.0479 (15)	0.0483 (15)	−0.0034 (12)	0.0069 (13)	−0.0073 (13)
C23A	0.0493 (16)	0.0656 (18)	0.0462 (16)	0.0028 (13)	0.0029 (13)	−0.0111 (14)
C24A	0.069 (2)	0.079 (2)	0.083 (2)	−0.0044 (17)	0.0165 (18)	−0.0340 (19)
C31A	0.0431 (14)	0.0350 (12)	0.0407 (14)	−0.0028 (11)	0.0059 (11)	−0.0002 (11)
C32A	0.0490 (15)	0.0422 (14)	0.0531 (16)	0.0000 (12)	0.0153 (13)	−0.0013 (12)
C33A	0.0730 (19)	0.0462 (15)	0.0560 (17)	−0.0051 (14)	0.0199 (15)	−0.0043 (13)
C34A	0.093 (2)	0.0500 (16)	0.066 (2)	0.0072 (16)	0.0276 (18)	−0.0101 (15)
C41A	0.0349 (13)	0.0385 (13)	0.0484 (15)	−0.0028 (10)	0.0051 (11)	0.0016 (11)
C42A	0.0430 (14)	0.0421 (13)	0.0452 (14)	−0.0035 (11)	0.0031 (12)	0.0019 (12)
C43A	0.0399 (14)	0.0529 (16)	0.0579 (17)	0.0005 (12)	0.0032 (13)	0.0000 (13)
C44A	0.0508 (17)	0.0596 (17)	0.0685 (19)	0.0023 (14)	−0.0082 (15)	0.0051 (15)

N2	0.0394 (11)	0.0412 (11)	0.0523 (13)	−0.0026 (9)	0.0149 (10)	0.0011 (10)
C11B	0.041 (4)	0.037 (4)	0.054 (6)	−0.007 (3)	0.022 (4)	0.004 (4)
C12B	0.069 (5)	0.046 (3)	0.045 (5)	−0.004 (3)	0.017 (4)	−0.005 (3)
C13B	0.106 (5)	0.058 (4)	0.063 (5)	−0.011 (3)	0.029 (5)	−0.011 (4)
C14B	0.153 (7)	0.069 (4)	0.106 (6)	0.009 (4)	0.047 (5)	−0.006 (4)
C11C	0.064 (9)	0.037 (7)	0.056 (10)	−0.010 (6)	0.033 (7)	0.000 (7)
C12C	0.059 (7)	0.052 (6)	0.038 (8)	−0.008 (5)	0.005 (7)	0.005 (5)
C13C	0.089 (7)	0.039 (6)	0.048 (7)	0.001 (5)	0.008 (7)	−0.007 (5)
C14C	0.101 (8)	0.076 (7)	0.078 (7)	−0.005 (6)	0.035 (6)	−0.031 (6)
C21B	0.0386 (14)	0.0501 (15)	0.0592 (17)	0.0017 (12)	0.0132 (13)	0.0060 (13)
C22B	0.0532 (18)	0.0639 (19)	0.089 (2)	0.0089 (15)	0.0155 (17)	0.0235 (18)
C23B	0.0566 (19)	0.084 (2)	0.088 (2)	0.0223 (17)	0.0136 (18)	0.022 (2)
C24D	0.068 (2)	0.108 (3)	0.083 (3)	0.007 (2)	0.004 (2)	0.025 (2)
C31B	0.0462 (15)	0.0426 (14)	0.0448 (14)	−0.0034 (11)	0.0144 (12)	0.0032 (12)
C32B	0.0491 (16)	0.0590 (16)	0.0508 (16)	−0.0009 (13)	0.0094 (13)	0.0038 (14)
C33B	0.0589 (18)	0.0642 (18)	0.0552 (17)	0.0073 (15)	0.0112 (14)	0.0100 (15)
C34B	0.085 (2)	0.0587 (19)	0.086 (2)	0.0119 (17)	0.015 (2)	0.0084 (18)
C41B	0.0421 (14)	0.0479 (15)	0.0461 (15)	0.0006 (12)	0.0135 (12)	0.0061 (12)
C42B	0.0518 (16)	0.0629 (18)	0.0613 (18)	−0.0039 (14)	0.0170 (15)	−0.0074 (15)
C43B	0.0580 (17)	0.0592 (17)	0.0432 (15)	0.0079 (14)	0.0093 (14)	0.0002 (13)
C44B	0.082 (2)	0.084 (2)	0.073 (2)	0.0012 (19)	0.0229 (19)	−0.0195 (19)

Geometric parameters (Å, °)

S1A—C1A	1.674 (3)	C41A—C42A	1.515 (3)
O1A—C2A	1.359 (3)	C41A—H41A	0.99
O1A—C1A	1.413 (3)	C41A—H41B	0.99
O2A—C4A	1.351 (3)	C42A—C43A	1.517 (3)
O2A—H2A	0.90 (3)	C42A—H42A	0.99
N1A—C1A	1.312 (3)	C42A—H42B	0.99
N1A—N2A	1.408 (3)	C43A—C44A	1.519 (4)
N2A—C2A	1.287 (3)	C43A—H43A	0.99
C2A—C3A	1.446 (3)	C43A—H43B	0.99
C3A—C8A	1.394 (3)	C44A—H44A	0.98
C3A—C4A	1.403 (4)	C44A—H44B	0.98
C4A—C5A	1.394 (4)	C44A—H44C	0.98
C5A—C6A	1.382 (4)	N2—C31B	1.516 (3)
C5A—H5A	0.95	N2—C41B	1.522 (3)
C6A—C7A	1.372 (4)	N2—C21B	1.522 (3)
C6A—H6A	0.95	N2—C11B	1.524 (5)
C7A—C8A	1.379 (4)	N2—C11C	1.526 (8)
C7A—H7A	0.95	C11B—C12B	1.523 (6)
C8A—H8A	0.95	C11B—H11C	0.99
S1B—C1B	1.684 (2)	C11B—H11D	0.99
O1B—C2B	1.356 (3)	C12B—C13B	1.534 (5)
O1B—C1B	1.405 (3)	C12B—H12C	0.99
O2B—C4B	1.360 (3)	C12B—H12D	0.99
O2B—H2B	0.87 (3)	C13B—C14B	1.504 (6)
N1B—C1B	1.308 (3)	C13B—H13C	0.99

N1B—N2B	1.410 (3)	C13B—H13D	0.99
N2B—C2B	1.290 (3)	C14B—H14D	0.98
C2B—C3B	1.451 (3)	C14B—H14E	0.98
C3B—C8B	1.393 (3)	C14B—H14F	0.98
C3B—C4B	1.404 (3)	C11C—C12C	1.521 (8)
C4B—C5B	1.386 (3)	C11C—H11E	0.99
C5B—C6B	1.375 (4)	C11C—H11F	0.99
C5B—H5B	0.95	C12C—C13C	1.527 (7)
C6B—C7B	1.387 (4)	C12C—H12E	0.99
C6B—H6B	0.95	C12C—H12F	0.99
C7B—C8B	1.381 (3)	C13C—C14C	1.510 (7)
C7B—H7B	0.95	C13C—H13E	0.99
C8B—H8B	0.95	C13C—H13F	0.99
N1—C21A	1.513 (3)	C14C—H14G	0.98
N1—C31A	1.517 (3)	C14C—H14H	0.98
N1—C41A	1.521 (3)	C14C—H14I	0.98
N1—C11A	1.523 (3)	C21B—C22B	1.518 (4)
C11A—C12A	1.516 (3)	C21B—H21C	0.99
C11A—H11A	0.99	C21B—H21D	0.99
C11A—H11B	0.99	C22B—C23B	1.528 (4)
C12A—C13A	1.511 (4)	C22B—H22C	0.99
C12A—H12A	0.99	C22B—H22D	0.99
C12A—H12B	0.99	C23B—C24D	1.508 (5)
C13A—C14A	1.518 (4)	C23B—H23C	0.99
C13A—H13A	0.99	C23B—H23D	0.99
C13A—H13B	0.99	C24D—H24D	0.98
C14A—H14A	0.98	C24D—H24E	0.98
C14A—H14B	0.98	C24D—H24F	0.98
C14A—H14C	0.98	C31B—C32B	1.520 (3)
C21A—C22A	1.516 (3)	C31B—H31C	0.99
C21A—H21A	0.99	C31B—H31D	0.99
C21A—H21B	0.99	C32B—C33B	1.530 (4)
C22A—C23A	1.521 (4)	C32B—H32C	0.99
C22A—H22A	0.99	C32B—H32D	0.99
C22A—H22B	0.99	C33B—C34B	1.515 (4)
C23A—C24A	1.524 (4)	C33B—H33C	0.99
C23A—H23A	0.99	C33B—H33D	0.99
C23A—H23B	0.99	C34B—H34D	0.98
C24A—H24A	0.98	C34B—H34E	0.98
C24A—H24B	0.98	C34B—H34F	0.98
C24A—H24C	0.98	C41B—C42B	1.516 (3)
C31A—C32A	1.517 (3)	C41B—H41C	0.99
C31A—H31A	0.99	C41B—H41D	0.99
C31A—H31B	0.99	C42B—C43B	1.513 (4)
C32A—C33A	1.513 (3)	C42B—H42C	0.99
C32A—H32A	0.99	C42B—H42D	0.99
C32A—H32B	0.99	C43B—C44B	1.508 (4)
C33A—C34A	1.523 (4)	C43B—H43C	0.99
C33A—H33A	0.99	C43B—H43D	0.99

C33A—H33B	0.99	C44B—H44D	0.98
C34A—H34A	0.98	C44B—H44E	0.98
C34A—H34B	0.98	C44B—H44F	0.98
C34A—H34C	0.98		
C2A—O1A—C1A	103.44 (18)	C43A—C42A—H42A	109.8
C4A—O2A—H2A	108 (2)	C41A—C42A—H42B	109.8
C1A—N1A—N2A	107.08 (19)	C43A—C42A—H42B	109.8
C2A—N2A—N1A	107.33 (19)	H42A—C42A—H42B	108.3
N1A—C1A—O1A	109.6 (2)	C42A—C43A—C44A	113.0 (2)
N1A—C1A—S1A	130.76 (19)	C42A—C43A—H43A	109.0
O1A—C1A—S1A	119.60 (17)	C44A—C43A—H43A	109.0
N2A—C2A—O1A	112.5 (2)	C42A—C43A—H43B	109.0
N2A—C2A—C3A	127.3 (2)	C44A—C43A—H43B	109.0
O1A—C2A—C3A	120.2 (2)	H43A—C43A—H43B	107.8
C8A—C3A—C4A	119.2 (2)	C43A—C44A—H44A	109.5
C8A—C3A—C2A	121.5 (2)	C43A—C44A—H44B	109.5
C4A—C3A—C2A	119.3 (2)	H44A—C44A—H44B	109.5
O2A—C4A—C5A	118.3 (3)	C43A—C44A—H44C	109.5
O2A—C4A—C3A	122.3 (2)	H44A—C44A—H44C	109.5
C5A—C4A—C3A	119.4 (3)	H44B—C44A—H44C	109.5
C6A—C5A—C4A	120.0 (3)	C31B—N2—C41B	110.88 (18)
C6A—C5A—H5A	120.0	C31B—N2—C21B	106.03 (18)
C4A—C5A—H5A	120.0	C41B—N2—C21B	110.9 (2)
C7A—C6A—C5A	120.9 (3)	C31B—N2—C11B	108.3 (7)
C7A—C6A—H6A	119.6	C41B—N2—C11B	109.4 (5)
C5A—C6A—H6A	119.6	C21B—N2—C11B	111.3 (7)
C6A—C7A—C8A	119.8 (3)	C12B—C11B—N2	119.6 (6)
C6A—C7A—H7A	120.1	C12B—C11B—H11C	107.4
C8A—C7A—H7A	120.1	N2—C11B—H11C	107.4
C7A—C8A—C3A	120.8 (3)	C12B—C11B—H11D	107.4
C7A—C8A—H8A	119.6	N2—C11B—H11D	107.4
C3A—C8A—H8A	119.6	H11C—C11B—H11D	106.9
C2B—O1B—C1B	103.65 (17)	C11B—C12B—C13B	113.1 (6)
C4B—O2B—H2B	113 (2)	C11B—C12B—H12C	109.0
C1B—N1B—N2B	107.19 (18)	C13B—C12B—H12C	109.0
C2B—N2B—N1B	106.85 (18)	C11B—C12B—H12D	109.0
N1B—C1B—O1B	109.81 (19)	C13B—C12B—H12D	109.0
N1B—C1B—S1B	130.57 (18)	H12C—C12B—H12D	107.8
O1B—C1B—S1B	119.61 (16)	C14B—C13B—C12B	112.6 (6)
N2B—C2B—O1B	112.5 (2)	C14B—C13B—H13C	109.1
N2B—C2B—C3B	126.9 (2)	C12B—C13B—H13C	109.1
O1B—C2B—C3B	120.6 (2)	C14B—C13B—H13D	109.1
C8B—C3B—C4B	119.0 (2)	C12B—C13B—H13D	109.1
C8B—C3B—C2B	122.0 (2)	H13C—C13B—H13D	107.8
C4B—C3B—C2B	119.0 (2)	C13B—C14B—H14D	109.5
O2B—C4B—C5B	118.0 (2)	C13B—C14B—H14E	109.5
O2B—C4B—C3B	122.2 (2)	H14D—C14B—H14E	109.5
C5B—C4B—C3B	119.7 (2)	C13B—C14B—H14F	109.5
C6B—C5B—C4B	120.3 (2)	H14D—C14B—H14F	109.5

C6B—C5B—H5B	119.8	H14E—C14B—H14F	109.5
C4B—C5B—H5B	119.8	C12C—C11C—N2	107.1 (12)
C5B—C6B—C7B	120.6 (3)	C12C—C11C—H11E	110.3
C5B—C6B—H6B	119.7	N2—C11C—H11E	110.3
C7B—C6B—H6B	119.7	C12C—C11C—H11F	110.3
C8B—C7B—C6B	119.5 (3)	N2—C11C—H11F	110.3
C8B—C7B—H7B	120.2	H11E—C11C—H11F	108.5
C6B—C7B—H7B	120.2	C11C—C12C—C13C	106.3 (10)
C7B—C8B—C3B	120.8 (2)	C11C—C12C—H12E	110.5
C7B—C8B—H8B	119.6	C13C—C12C—H12E	110.5
C3B—C8B—H8B	119.6	C11C—C12C—H12F	110.5
C21A—N1—C31A	105.77 (17)	C13C—C12C—H12F	110.5
C21A—N1—C41A	111.64 (18)	H12E—C12C—H12F	108.7
C31A—N1—C41A	111.14 (17)	C14C—C13C—C12C	112.6 (11)
C21A—N1—C11A	111.74 (18)	C14C—C13C—H13E	109.1
C31A—N1—C11A	111.30 (17)	C12C—C13C—H13E	109.1
C41A—N1—C11A	105.37 (17)	C14C—C13C—H13F	109.1
C12A—C11A—N1	116.12 (19)	C12C—C13C—H13F	109.1
C12A—C11A—H11A	108.3	H13E—C13C—H13F	107.8
N1—C11A—H11A	108.3	C13C—C14C—H14G	109.5
C12A—C11A—H11B	108.3	C13C—C14C—H14H	109.5
N1—C11A—H11B	108.3	H14G—C14C—H14H	109.5
H11A—C11A—H11B	107.4	C13C—C14C—H14I	109.5
C13A—C12A—C11A	110.4 (2)	H14G—C14C—H14I	109.5
C13A—C12A—H12A	109.6	H14H—C14C—H14I	109.5
C11A—C12A—H12A	109.6	C22B—C21B—N2	115.4 (2)
C13A—C12A—H12B	109.6	C22B—C21B—H21C	108.4
C11A—C12A—H12B	109.6	N2—C21B—H21C	108.4
H12A—C12A—H12B	108.1	C22B—C21B—H21D	108.4
C12A—C13A—C14A	112.7 (3)	N2—C21B—H21D	108.4
C12A—C13A—H13A	109.1	H21C—C21B—H21D	107.5
C14A—C13A—H13A	109.1	C21B—C22B—C23B	110.9 (2)
C12A—C13A—H13B	109.1	C21B—C22B—H22C	109.5
C14A—C13A—H13B	109.1	C23B—C22B—H22C	109.5
H13A—C13A—H13B	107.8	C21B—C22B—H22D	109.5
C13A—C14A—H14A	109.5	C23B—C22B—H22D	109.5
C13A—C14A—H14B	109.5	H22C—C22B—H22D	108.0
H14A—C14A—H14B	109.5	C24D—C23B—C22B	112.6 (3)
C13A—C14A—H14C	109.5	C24D—C23B—H23C	109.1
H14A—C14A—H14C	109.5	C22B—C23B—H23C	109.1
H14B—C14A—H14C	109.5	C24D—C23B—H23D	109.1
N1—C21A—C22A	116.4 (2)	C22B—C23B—H23D	109.1
N1—C21A—H21A	108.2	H23C—C23B—H23D	107.8
C22A—C21A—H21A	108.2	C23B—C24D—H24D	109.5
N1—C21A—H21B	108.2	C23B—C24D—H24E	109.5
C22A—C21A—H21B	108.2	H24D—C24D—H24E	109.5
H21A—C21A—H21B	107.3	C23B—C24D—H24F	109.5
C21A—C22A—C23A	109.4 (2)	H24D—C24D—H24F	109.5
C21A—C22A—H22A	109.8	H24E—C24D—H24F	109.5

C23A—C22A—H22A	109.8	N2—C31B—C32B	115.8 (2)
C21A—C22A—H22B	109.8	N2—C31B—H31C	108.3
C23A—C22A—H22B	109.8	C32B—C31B—H31C	108.3
H22A—C22A—H22B	108.2	N2—C31B—H31D	108.3
C22A—C23A—C24A	112.1 (2)	C32B—C31B—H31D	108.3
C22A—C23A—H23A	109.2	H31C—C31B—H31D	107.4
C24A—C23A—H23A	109.2	C31B—C32B—C33B	110.9 (2)
C22A—C23A—H23B	109.2	C31B—C32B—H32C	109.5
C24A—C23A—H23B	109.2	C33B—C32B—H32C	109.4
H23A—C23A—H23B	107.9	C31B—C32B—H32D	109.4
C23A—C24A—H24A	109.5	C33B—C32B—H32D	109.4
C23A—C24A—H24B	109.5	H32C—C32B—H32D	108.0
H24A—C24A—H24B	109.5	C34B—C33B—C32B	114.2 (2)
C23A—C24A—H24C	109.5	C34B—C33B—H33C	108.7
H24A—C24A—H24C	109.5	C32B—C33B—H33C	108.7
H24B—C24A—H24C	109.5	C34B—C33B—H33D	108.7
N1—C31A—C32A	115.64 (19)	C32B—C33B—H33D	108.7
N1—C31A—H31A	108.4	H33C—C33B—H33D	107.6
C32A—C31A—H31A	108.4	C33B—C34B—H34D	109.5
N1—C31A—H31B	108.4	C33B—C34B—H34E	109.5
C32A—C31A—H31B	108.4	H34D—C34B—H34E	109.5
H31A—C31A—H31B	107.4	C33B—C34B—H34F	109.5
C33A—C32A—C31A	110.0 (2)	H34D—C34B—H34F	109.5
C33A—C32A—H32A	109.7	H34E—C34B—H34F	109.5
C31A—C32A—H32A	109.7	C42B—C41B—N2	115.9 (2)
C33A—C32A—H32B	109.7	C42B—C41B—H41C	108.3
C31A—C32A—H32B	109.7	N2—C41B—H41C	108.3
H32A—C32A—H32B	108.2	C42B—C41B—H41D	108.3
C32A—C33A—C34A	112.4 (2)	N2—C41B—H41D	108.3
C32A—C33A—H33A	109.1	H41C—C41B—H41D	107.4
C34A—C33A—H33A	109.1	C43B—C42B—C41B	109.8 (2)
C32A—C33A—H33B	109.1	C43B—C42B—H42C	109.7
C34A—C33A—H33B	109.1	C41B—C42B—H42C	109.7
H33A—C33A—H33B	107.9	C43B—C42B—H42D	109.7
C33A—C34A—H34A	109.5	C41B—C42B—H42D	109.7
C33A—C34A—H34B	109.5	H42C—C42B—H42D	108.2
H34A—C34A—H34B	109.5	C44B—C43B—C42B	113.6 (2)
C33A—C34A—H34C	109.5	C44B—C43B—H43C	108.8
H34A—C34A—H34C	109.5	C42B—C43B—H43C	108.8
H34B—C34A—H34C	109.5	C44B—C43B—H43D	108.8
C42A—C41A—N1	117.04 (19)	C42B—C43B—H43D	108.8
C42A—C41A—H41A	108.0	H43C—C43B—H43D	107.7
N1—C41A—H41A	108.0	C43B—C44B—H44D	109.5
C42A—C41A—H41B	108.0	C43B—C44B—H44E	109.5
N1—C41A—H41B	108.0	H44D—C44B—H44E	109.5
H41A—C41A—H41B	107.3	C43B—C44B—H44F	109.5
C41A—C42A—C43A	109.3 (2)	H44D—C44B—H44F	109.5
C41A—C42A—H42A	109.8	H44E—C44B—H44F	109.5
C1A—N1A—N2A—C2A	−0.3 (3)	C6B—C7B—C8B—C3B	−1.2 (5)

N2A—N1A—C1A—O1A	0.5 (3)	C4B—C3B—C8B—C7B	0.7 (4)
N2A—N1A—C1A—S1A	−178.8 (2)	C2B—C3B—C8B—C7B	−179.3 (3)
C2A—O1A—C1A—N1A	−0.5 (3)	C21A—N1—C11A—C12A	−65.0 (3)
C2A—O1A—C1A—S1A	178.96 (18)	C31A—N1—C11A—C12A	53.0 (3)
N1A—N2A—C2A—O1A	0.0 (3)	C41A—N1—C11A—C12A	173.5 (2)
N1A—N2A—C2A—C3A	−178.2 (2)	N1—C11A—C12A—C13A	176.6 (2)
C1A—O1A—C2A—N2A	0.2 (3)	C11A—C12A—C13A—C14A	166.0 (3)
C1A—O1A—C2A—C3A	178.7 (2)	C31A—N1—C21A—C22A	−176.2 (2)
N2A—C2A—C3A—C8A	−175.8 (3)	C41A—N1—C21A—C22A	62.8 (2)
O1A—C2A—C3A—C8A	6.1 (4)	C11A—N1—C21A—C22A	−54.9 (3)
N2A—C2A—C3A—C4A	6.2 (4)	N1—C21A—C22A—C23A	−168.78 (19)
O1A—C2A—C3A—C4A	−172.0 (2)	C21A—C22A—C23A—C24A	−171.3 (2)
C8A—C3A—C4A—O2A	−179.8 (2)	C21A—N1—C31A—C32A	−177.51 (19)
C2A—C3A—C4A—O2A	−1.7 (4)	C41A—N1—C31A—C32A	−56.2 (3)
C8A—C3A—C4A—C5A	0.7 (4)	C11A—N1—C31A—C32A	60.9 (3)
C2A—C3A—C4A—C5A	178.8 (3)	N1—C31A—C32A—C33A	−177.0 (2)
O2A—C4A—C5A—C6A	179.8 (3)	C31A—C32A—C33A—C34A	−177.7 (2)
C3A—C4A—C5A—C6A	−0.6 (4)	C21A—N1—C41A—C42A	58.0 (3)
C4A—C5A—C6A—C7A	0.3 (5)	C31A—N1—C41A—C42A	−59.8 (3)
C5A—C6A—C7A—C8A	0.1 (5)	C11A—N1—C41A—C42A	179.5 (2)
C6A—C7A—C8A—C3A	0.0 (5)	N1—C41A—C42A—C43A	170.3 (2)
C4A—C3A—C8A—C7A	−0.4 (4)	C41A—C42A—C43A—C44A	−179.5 (2)
C2A—C3A—C8A—C7A	−178.5 (3)	C31B—N2—C11B—C12B	−51.7 (14)
C1B—N1B—N2B—C2B	−0.2 (3)	C41B—N2—C11B—C12B	−172.7 (10)
N2B—N1B—C1B—O1B	0.1 (3)	C21B—N2—C11B—C12B	64.5 (14)
N2B—N1B—C1B—S1B	178.85 (19)	N2—C11B—C12B—C13B	−175.7 (11)
C2B—O1B—C1B—N1B	0.0 (2)	C11B—C12B—C13B—C14B	73.9 (12)
C2B—O1B—C1B—S1B	−178.86 (17)	N2—C11C—C12C—C13C	−177.2 (18)
N1B—N2B—C2B—O1B	0.3 (3)	C11C—C12C—C13C—C14C	−178.2 (18)
N1B—N2B—C2B—C3B	−178.7 (2)	C31B—N2—C21B—C22B	173.9 (2)
C1B—O1B—C2B—N2B	−0.2 (3)	C41B—N2—C21B—C22B	−65.7 (3)
C1B—O1B—C2B—C3B	178.8 (2)	C11B—N2—C21B—C22B	56.3 (6)
N2B—C2B—C3B—C8B	178.9 (2)	N2—C21B—C22B—C23B	161.1 (2)
O1B—C2B—C3B—C8B	0.0 (4)	C41B—N2—C31B—C32B	58.0 (3)
N2B—C2B—C3B—C4B	−1.1 (4)	C21B—N2—C31B—C32B	178.4 (2)
O1B—C2B—C3B—C4B	−180.0 (2)	C11B—N2—C31B—C32B	−62.0 (6)
C8B—C3B—C4B—O2B	179.4 (2)	N2—C31B—C32B—C33B	−175.4 (2)
C2B—C3B—C4B—O2B	−0.7 (4)	C31B—C32B—C33B—C34B	67.5 (3)
C8B—C3B—C4B—C5B	0.2 (4)	C31B—N2—C41B—C42B	57.2 (3)
C2B—C3B—C4B—C5B	−179.8 (2)	C21B—N2—C41B—C42B	−60.3 (3)
O2B—C4B—C5B—C6B	−179.8 (2)	C11B—N2—C41B—C42B	176.6 (8)
C3B—C4B—C5B—C6B	−0.7 (4)	N2—C41B—C42B—C43B	−179.5 (2)
C4B—C5B—C6B—C7B	0.2 (4)	C41B—C42B—C43B—C44B	−175.9 (2)
C5B—C6B—C7B—C8B	0.7 (5)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2A—H2A···N2A	0.90 (3)	1.86 (3)	2.665 (3)	148 (3)

O2B—H2B···N2B	0.87 (3)	1.90 (3)	2.645 (3)	143 (3)
C11B—H11C···N1B^{i}	0.99	2.47	3.440 (16)	165
C21A—H21A···N1B^{i}	0.99	2.57	3.551 (3)	172
C31B—H31D···O2B	0.99	2.58	3.511 (3)	157
C41A—H41B···S1B^{ii}	0.99	2.79	3.520 (3)	131
C11C—H11E···N1B^{i}	0.99	2.42	3.38 (3)	163
C41B—H41C···N1A	0.99	2.52	3.459 (3)	157
C24B—H24E···Cg1	0.99	2.92	3.863 (3)	159
C42A—H42B···Cg2^{iii}	0.99	2.93	3.576 (3)	125

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) *x*+1/2, −*y*+3/2, *z*−1/2; (iii) −*x*+3/2, *y*+1/2, −*z*+1/2.

Fig. 1

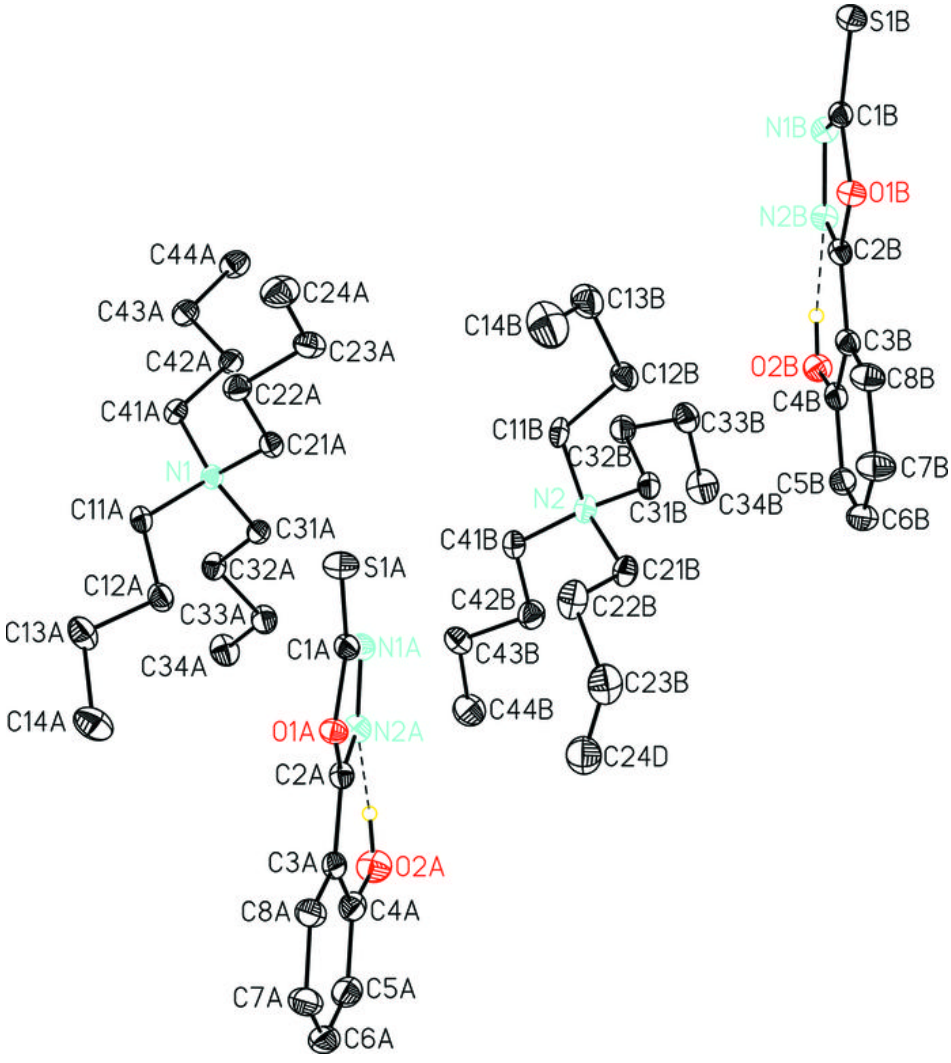

S1B
C1B
N1B
O1B
N2B
C2B
C3B
O2B
C8B
C4B
C7B
C5B
C6B
C13B
C14B
C12B
C11B
C33B
C32B
N2
C31B
C34B
C41B
C21B
C42B
C22B
C43B
C23B
C44B
C24D
C44A
C24A
C43A
C23A
C42A
C22A
C41A
C21A
N1
C11A
C31A
C32A
S1A
C12A
C33A
C13A
C1A
N1A
C34A
C14A
O1A
N2A
C2A
C3A
O2A
C8A
C4A
C7A
C5A
C6A

Fig. 2