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Bis{4-[(*Z*)-*N*′-(4-hydroxybenzylidene)-hydrazino]-8-(trifluoromethyl)-quinolinium} sulfate dihydrate

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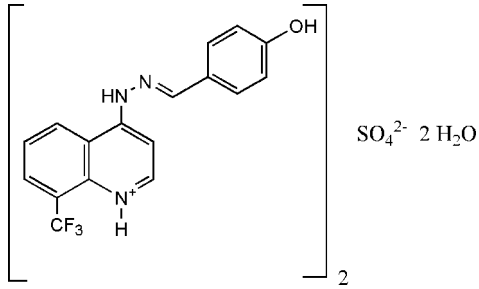
Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.002 Å; R factor = 0.043; wR factor = 0.128; data-to-parameter ratio = 13.5.

The title compound, $2C_{17}H_{13}F_3N_3O^+\cdot SO_4^{2-}\cdot 2H_2O$, crystallizes with four independent cations (*A*, *B*, *C* and *D*) in the asymmetric unit, which is composed of two groups of two cations, one anion and two water molecules (Z' = 2). The dihedral angle between the mean planes of the 4-hydroxyphenyl and quinolinium groups is 8.9 (7)° in *A*, 30.1 (6)° in *B*, 28.8 (8)° in *C* and 12.8 (1)° in *D*. The crystal packing is stabilized by intermolecular O—H···O and N—H···O hydrogen bonding between H atoms from 4-hydroxyphenyl O atoms and the O atoms of nearby water molecules and sulfate anions, as well as H atoms from the N atom of the hydrazino group to O atoms of neighboring sulfate anions, linking the components into chains with the 4-hydroxyphenyl and quinolinium rings parallel to the (011) plane. There is also an extensive array of intermolecular hydrogen bonds between water molecules themselves and with sulfate O atoms, as well as hydrogen-bond interactions between H atoms from the hydrazino group and sulfate O atoms. In addition, intermolecular π–π stacking interactions occur between nearby 4-hydroxyphenyl and quinolinium groups, with distances between the centroids of interacting rings in the range 3.4140 (9)–3.9659 (9) Å.

Related literature

For related structures, see: Yathirajan *et al.* (2007); Fun *et al.* (1999); Wang *et al.* (1998); Sadık *et al.* (2004). For related literature, see: Roma *et al.* (2000); Chen *et al.* (2001); Maguire *et al.* (1994); Zhang *et al.* (2000); Kahwa *et al.* (1986); Santos *et al.* (2001); Saim *et al.* (2004); El-Masry *et al.* (2000); Pandey *et al.* (1999); Hodnett *et al.* (1970); Misra *et al.* (1981); Varma *et al.* (1986); Singh *et al.* (1988); Desai *et al.* (2001).



Experimental

Crystal data

$2C_{17}H_{13}F_3N_3O^+\cdot SO_4^{2-}\cdot 2H_2O$
M_r = 796.70
Monoclinic, $P2_1/a$
a = 13.4349 (1) Å
b = 23.8601 (1) Å
c = 21.7174 (1) Å
β = 96.8568 (4)°
V = 6911.89 (7) Å^3
Z = 8
Cu $K\alpha$ radiation
μ = 1.68 mm^{-1}
T = 200 (2) K
0.55 × 0.37 × 0.19 mm

Data collection

Oxford Diffraction Gemini R CCD diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.441, T_{max} = 0.727
45529 measured reflections
13742 independent reflections
11290 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.127
S = 1.05
13742 reflections
1020 parameters
12 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.74 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O4*W*—H4*W*1···O11^{i}	0.835 (18)	2.23 (3)	2.986 (2)	151 (5)
N2*A*—H2*AB*···O11^{i}	0.88	1.99	2.8592 (18)	170
C4*A*—H4*AA*···O11^{i}	0.95	2.28	3.199 (2)	163
O1*A*—H1*A*···O12^{ii}	0.84	1.89	2.6677 (18)	154
O1*D*—H1*D*···O13^{ii}	0.84	1.75	2.5771 (17)	167
O4*W*—H4*W*2···O14^{iii}	0.820 (19)	2.06 (2)	2.860 (2)	167 (5)
C4*D*—H4*DA*···O14^{iii}	0.95	2.50	3.367 (2)	152
C11*D*—H11*D*···O14^{iii}	0.95	2.52	3.272 (2)	136
N1*A*—H1*AA*···O21^{i}	0.88	2.06	2.8636 (18)	151
O3*W*—H3*W*2···O22^{i}	0.841 (18)	2.039 (19)	2.864 (2)	167 (4)
N2*B*—H2*BB*···O22^{iv}	0.88	1.93	2.7909 (18)	166
C4*B*—H4*BA*···O22^{iv}	0.95	2.37	3.294 (2)	165
C11*B*—H11*B*···O22^{iv}	0.95	2.55	3.319 (2)	138
O3*W*—H3*W*1···O23^{iii}	0.824 (18)	1.952 (19)	2.776 (2)	179 (5)
O1*W*—H1*W*1···O24^{iii}	0.810 (17)	1.933 (17)	2.725 (2)	165 (3)
C8*A*—H8*AA*···O24^{i}	0.95	2.39	3.134 (2)	135
C7*C*—H7*CA*···O1*A*^{v}	0.95	2.46	3.0647 (19)	122
C8*C*—H8*CA*···O1*A*^{v}	0.95	2.47	3.078 (2)	122
O2*W*—H2*W*1···O1*D*^{vi}	0.821 (17)	2.114 (18)	2.933 (2)	175 (4)
C8*B*—H8*BA*···O1*D*^{v}	0.95	2.34	3.234 (2)	157
O1*C*—H1*C*···O3*W*^{v}	0.84	1.82	2.651 (2)	168
O2*W*—H2*W*2···O4*W*^{i}	0.828 (17)	1.931 (17)	2.759 (3)	177 (3)

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

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Data collection: *CrysAlisPro* (Oxford Diffraction, 2007); cell refinement: *CrysAlisPro*; data reduction: *CrysAlisPro*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NC2084).

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supplementary materials

Acta Cryst. (2008). E**64**, o481-o482 [**doi:10.1107/S1600536808000561**]

Bis{4-[(*Z*)-*N*'-(4-hydroxybenzylidene)hydrazino]-8-(trifluoromethyl)quinolinium} sulfate dihydrate

J. P. Jasinski, R. J. Butcher, B. Narayana, K. Sunil and H. S. Yathirajan

Comment

It is well known that the quinoline ring system is an important structural unit widely existing in alkaloids, therapeutics and synthetic analogues with interesting biological activities (Roma *et al.* 2000 and Chen *et al.* 2001). A large variety of quinoline derivatives have been used as antimalarial, anti-inflammatory agents, antiasthmatic, antibacterial, antihypertensive and tyrokinase PDGF-RTK inhibiting agents (Maguire *et al.* 1994). Furthermore, poly-substituted quinolines have been found to undergo hierarchical self-assembly into a variety of nano- and mesostructures with enhanced electronic and photonic functions (Zhang *et al.* 2000). The synthesis and structure of Schiff bases have attracted much attention in biology and chemistry (Kahwa *et al.* 1986). One of the aims of investigating the structural chemistry of Schiff bases is to develop protein and enzyme mimics (Santos *et al.* 2001). Structural information is useful in investigating the coordination properties of Schiff bases functioning as ligands (Saim *et al.* 2004). Some Schiff base derivatives were reported to possess antimicrobial, anti-inflammatory and central nervous system activities. Moreover, Schiff bases are also known to have biological activities such as antimicrobial (El-Masry *et al.*. 2000 & Pandey *et al.* 1999), antifungal (Singh *et al*. 1988 & Varma *et al.* 1986), antitumor (Hodnett *et al*. 1970; Misra *et al.* 1981 & Desai *et al.* 2001), and as herbicides. The crystal structures of Schiff base compounds, *viz*, bis{4-[(2-hydroxybenzylidine)hydrazino]-8-(trifluoromethyl)quinolinium} sulfate tetrahydrate, (Yathirajan *et al.* 2007), *p*-hydroxybenzaldehyde nicotinoylhydrazone monohydrate (Fun *et al.* 1999), 2-(2-hydroxybenzylidene)-1-(2-picoloyl)hydrazine hemihydrate (Wang *et al.* 1998), 5-bromo-2-hydroxybenzaldehyde (4-phenyl-1,3-thiazol-2-yl)hydrazone (Sadık *et al.* 2004) have been reported. A new Schiff base, $C_{34}H_{30}F_6N_6O_8S$, was synthesized and its crystal structure is reported.

The title compound, $C_{34}H_{30}F_6N_6O_8S$, crystallizes with four independent cations (A, B, C and D) in the asymmetric unit which is composed of two groups of two cations, one anion and two water molecules [*Z*'= 2], respectively (Figs. 1–2). The dihedral angle between the mean planes of the 4-hydroxyphenyl and quinolinium groups is 8.9 (7)° in A, 30.1 (6)° in B, 28.8 (8)° in C and 12.8 (1)° in D. Crystal packing is stabilized by intermolecular O—H···O and N—H···O hydrogen bonding between H atoms from 4-hydroxyphenyl oxygen atoms and oxygen atoms from nearby water and sulfate molecules as well as H atoms from the nitrogen atom of the hydrazino group to oxygen atoms from neighboring sulfate molecules linking the molecules into chains with the 4-hydroxyphenyl and quinolimium rings parallel to the [011] plane of the unit cell (Fig. 3). There is also an extensive array of intermolecular hydrogen bonds between water molecules themselves and with sulfate oxygen atoms,in the unit cell as well as hydrogen bond interactions between hydrogen atoms from the hydrazino group and sulfate oxygen atoms. Also, intermolecular π-π stacking interactions occur between adjacent 4-hydroxyphenyl and quinolinium rings as follows: [*Cg*1, *Cg*2, *Cg*3, *Cg*5, *Cg*6, *Cg*9, *Cg*10, *Cg*13, *Cg*14 & *Cg*15 = center of gravity of (N1A, C5A–C9A), (C1A–C5A, C9A), (C12A–C17A), (N1B, C5B–C9B), (C1B–C5B, C9B), (N1C, C5C–C9C), (C1C–C5C, C9C), (N1C, C5C–C9C), (C1D–C5D, C9D), (C12D–C17D); *Cg*1···*Cg*13 = 3.7262 (9) & 3.4140 (9)^{ix} Å; *Cg*2···*Cg*13 = 3.5888 (9)^{ix} Å; *Cg*2···*Cg*14 = 3.9659 (9)^{ix} Å; *Cg*3···*Cg*15 = 3.9401 (10)^{ix} Å; *Cg*5···*Cg*9 = 3.5848 (8)^{ix} & 3.6314 (9)^{x} Å; *Cg*6···*Cg*9 = 3.8223 (9)^{ix} & 3.5486 (9)^{x} Å; *Cg*6···*Cg*10 = 3.6649 (9)^{xi} Å; ix = *x*, *y*, *z*; *x* = 1/2 − *x*, 1/2 − *y*, *z*; xi = −1/2 + *x*, 1/2 − *y*, *z*].

Experimental

A mixture of 4-hydrazino-8-(trifluoromethyl)quinoline (1.135 g, 0.005 mol) and 4-hydroxybenzaldehyde (0.61 g, 0.005 mol) in 15 ml of absolute alcohol containing 2 drops of sulfuric acid was refluxed for about 3 h. On cooling, the solid separated, was filtered and recrystallized from DMF (m.p.: Above 523 K).

Refinement

The hydroxyl hydrogen atoms (H1A, H1B, H1C, H1D) and the amine hydrogen atoms (H1AA, H2AB, H1BA, H2BB, H1CA, H2CB, H1DA, H2DB) were located in a difference Fourier map and refined using the riding model with O—H = 0.84 Å, N—H = 0.88 Å. All other H atoms in cations A, B, C & D were placed in their calculated positions and then refined using the riding model with C—H = 0.95 Å, and with U_{iso}(H) = 1.18–1.21U_{eq}(C, N, O). O–H bonds and H–H distances in each of the water molecules were refined with restraints at 0.82 Å and 1.297 Å, respectively.

Figures

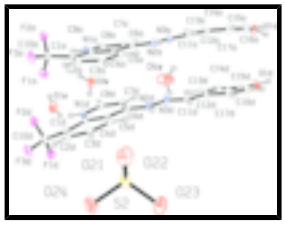


Fig. 1. Molecular structure of molecules A & D, a sulfate ion and 3 water molecules in a partial description of the asymmetric unit for the title compound, showing atom labeling and 30% probability displacement ellipsoids.

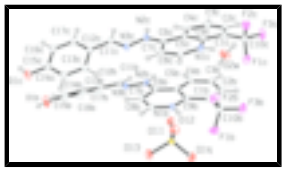


Fig. 2. Molecular structure of molecules B & C, a sulfate ion and 1 water molecule in a partial description of the asymmetric unit for the title compound, showing atom labeling and 30% probability displacement ellipsoids.

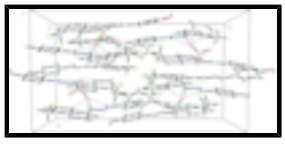


Fig. 3. Packing diagram of the title compound, viewed down the *c* axis. Dashed lines indicate intermolecular O—H···O and N—H···O hydrogen bonds.

Bis{4-[(*Z*)-*N*'-(4-hydroxybenzylidene)hydrazino]-8-\ (trifluoromethyl)quinolinium} sulfate dihydrate

Crystal data

$2C_{17}H_{13}F_3N_3O^+·S_1O_4^{2-}·2H_2O$	F_{000} = 3280
M_r = 796.70	D_x = 1.531 Mg m^{-3}
Monoclinic, $P2_1/a$	Cu $K\alpha$ radiation λ = 1.54184 Å
Hall symbol: -P 2yab	Cell parameters from 28034 reflections
a = 13.4349 (1) Å	θ = 4.1–73.8º
b = 23.8601 (1) Å	μ = 1.68 mm^{-1}
c = 21.7174 (1) Å	T = 200 (2) K

$\beta = 96.8568\ (4)^{o}$	Thick plate, yellow
$V = 6911.89\ (7)\ Å^3$	0.55 × 0.37 × 0.19 mm
$Z = 8$	

Data collection

Oxford Diffraction Gemini R CCD diffractometer	13742 independent reflections
Radiation source: fine-focus sealed tube	11290 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.026$
Detector resolution: 10.5081 pixels mm^{-1}	$\theta_{max} = 74.1^{o}$
$T = 200(2)$ K	$\theta_{min} = 4.1^{o}$
φ and ω scans	$h = -16 \rightarrow 15$
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2007)	$k = -29 \rightarrow 29$
$T_{min} = 0.441$, $T_{max} = 0.727$	$l = -27 \rightarrow 27$
45529 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
$R[F^2 > 2\sigma(F^2)] = 0.043$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.127$	$w = 1/[\sigma^2(F_o^2) + (0.0961P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} = 0.001$
13742 reflections	$\Delta\rho_{max} = 0.74$ e $Å^{-3}$
1020 parameters	$\Delta\rho_{min} = -0.41$ e $Å^{-3}$
12 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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}
S1	0.66689 (3)	0.187616 (15)	0.499522 (16)	0.02836 (10)
S2	0.75736 (3)	0.264569 (16)	0.980196 (16)	0.03112 (10)
F1A	0.38287 (9)	0.60885 (6)	0.16001 (6)	0.0492 (3)
F2A	0.23142 (8)	0.62688 (5)	0.17582 (6)	0.0456 (3)
F3A	0.30734 (11)	0.55656 (5)	0.22072 (6)	0.0549 (3)
F1B	0.77439 (9)	0.30958 (6)	0.39611 (5)	0.0505 (3)
F2B	0.61525 (9)	0.32051 (5)	0.38017 (5)	0.0454 (3)
F3B	0.71268 (11)	0.39064 (5)	0.37049 (6)	0.0528 (3)
F1C	0.52317 (9)	0.42538 (5)	0.29453 (6)	0.0497 (3)
F2C	0.36467 (9)	0.43361 (5)	0.27143 (7)	0.0504 (3)
F3C	0.46481 (11)	0.48564 (5)	0.22683 (7)	0.0548 (3)
F1D	0.72434 (11)	0.57600 (6)	0.15532 (6)	0.0581 (3)
F2D	0.56809 (9)	0.55653 (5)	0.14721 (5)	0.0463 (3)
F3D	0.67439 (11)	0.49953 (5)	0.19391 (6)	0.0552 (3)
O1A	0.48294 (10)	1.15354 (5)	0.36284 (6)	0.0369 (3)
H1A	0.5222	1.1637	0.3938	0.044*
O1B	0.82685 (15)	−0.10351 (6)	−0.01295 (9)	0.0600 (4)
H1B	0.8211	−0.1274	0.0149	0.072*
O1C	0.51549 (11)	−0.12665 (6)	0.14066 (7)	0.0439 (3)
H1C	0.5018	−0.1442	0.1072	0.053*
O1D	0.72708 (11)	1.07763 (5)	0.40646 (6)	0.0399 (3)
H1D	0.7263	1.0910	0.4422	0.048*
O11	0.57717 (10)	0.19361 (6)	0.53218 (6)	0.0402 (3)
O12	0.63883 (10)	0.19895 (5)	0.43294 (5)	0.0365 (3)
O13	0.70470 (11)	0.12950 (5)	0.50799 (6)	0.0411 (3)
O14	0.74565 (10)	0.22713 (5)	0.52553 (6)	0.0391 (3)
O21	0.70265 (11)	0.30509 (5)	0.93705 (6)	0.0419 (3)
O22	0.68867 (11)	0.24572 (6)	1.02472 (6)	0.0435 (3)
O23	0.84557 (12)	0.29237 (7)	1.01441 (6)	0.0494 (3)
O24	0.78908 (12)	0.21622 (6)	0.94591 (7)	0.0490 (3)
O1W	0.53785 (14)	0.66106 (7)	0.06907 (7)	0.0520 (4)
H1W1	0.5842 (17)	0.6790 (13)	0.0585 (16)	0.078*
H1W2	0.4867 (15)	0.6696 (15)	0.0473 (15)	0.078*
O2W	0.39849 (12)	0.35357 (7)	0.38120 (7)	0.0516 (4)
H2W1	0.353 (2)	0.3742 (12)	0.3894 (15)	0.077*
H2W2	0.410 (2)	0.3341 (13)	0.4128 (12)	0.077*
O3W	0.48321 (15)	0.80476 (10)	0.04431 (11)	0.0758 (6)
H3W1	0.5343 (19)	0.802 (2)	0.0270 (19)	0.114*
H3W2	0.438 (2)	0.7906 (19)	0.0191 (17)	0.114*
O4W	0.56157 (16)	0.71447 (10)	0.51613 (13)	0.0818 (7)
H4W1	0.532 (3)	0.7452 (12)	0.515 (2)	0.123*
H4W2	0.6178 (18)	0.7226 (18)	0.508 (2)	0.123*
N1A	0.34199 (10)	0.72867 (6)	0.18977 (6)	0.0309 (3)
H1AA	0.3257	0.7068	0.1575	0.037*
N2A	0.40367 (10)	0.83468 (6)	0.33901 (6)	0.0296 (3)

H2AB	0.4118	0.8217	0.3772	0.036*
N3A	0.40772 (10)	0.89174 (6)	0.32737 (6)	0.0310 (3)
N1B	0.68578 (10)	0.22189 (6)	0.31392 (6)	0.0291 (3)
H1BA	0.6837	0.2300	0.3533	0.035*
N2B	0.69915 (10)	0.17935 (6)	0.13111 (6)	0.0279 (3)
H2BB	0.6984	0.2050	0.1019	0.034*
N3B	0.70759 (10)	0.12263 (6)	0.11726 (6)	0.0301 (3)
N1C	0.43842 (10)	0.31498 (6)	0.27005 (6)	0.0295 (3)
H1CA	0.4313	0.3398	0.2992	0.035*
N2C	0.44382 (10)	0.19512 (6)	0.13377 (6)	0.0300 (3)
H2CB	0.4341	0.2047	0.0944	0.036*
N3C	0.45725 (10)	0.13929 (6)	0.15104 (6)	0.0315 (3)
N1D	0.60597 (10)	0.67250 (6)	0.19298 (6)	0.0308 (3)
H1DA	0.5954	0.6544	0.1575	0.037*
N2D	0.65741 (10)	0.76047 (5)	0.35705 (6)	0.0280 (3)
H2DB	0.6703	0.7429	0.3928	0.034*
N3D	0.65647 (10)	0.81849 (5)	0.35395 (6)	0.0290 (3)
C1A	0.35732 (12)	0.64644 (7)	0.25706 (8)	0.0320 (3)
C2A	0.38460 (13)	0.62364 (7)	0.31475 (8)	0.0350 (3)
H2AA	0.3841	0.5841	0.3201	0.042*
C3A	0.41310 (13)	0.65853 (8)	0.36574 (8)	0.0349 (3)
H3AA	0.4333	0.6425	0.4053	0.042*
C4A	0.41202 (12)	0.71545 (7)	0.35901 (7)	0.0305 (3)
H4AA	0.4284	0.7387	0.3943	0.037*
C5A	0.38664 (11)	0.74009 (7)	0.29990 (7)	0.0266 (3)
C6A	0.38709 (11)	0.80012 (7)	0.29088 (7)	0.0274 (3)
C7A	0.36927 (12)	0.82069 (7)	0.22972 (7)	0.0314 (3)
H7AA	0.3724	0.8598	0.2221	0.038*
C8A	0.34752 (13)	0.78431 (8)	0.18157 (7)	0.0328 (3)
H8AA	0.3358	0.7989	0.1406	0.039*
C9A	0.36138 (11)	0.70516 (7)	0.24806 (7)	0.0286 (3)
C10A	0.32063 (13)	0.60916 (8)	0.20370 (9)	0.0369 (4)
C11A	0.41583 (13)	0.92246 (7)	0.37550 (8)	0.0337 (3)
H11A	0.4166	0.9056	0.4152	0.040*
C12A	0.42402 (12)	0.98322 (7)	0.37085 (7)	0.0320 (3)
C13A	0.41453 (13)	1.01174 (7)	0.31441 (7)	0.0335 (3)
H13A	0.3953	0.9920	0.2769	0.040*
C14A	0.43297 (13)	1.06857 (7)	0.31306 (7)	0.0346 (3)
H14A	0.4256	1.0878	0.2745	0.042*
C15A	0.46239 (12)	1.09814 (7)	0.36776 (7)	0.0301 (3)
C16A	0.46704 (15)	1.07083 (8)	0.42426 (8)	0.0397 (4)
H16A	0.4842	1.0908	0.4619	0.048*
C17A	0.44635 (16)	1.01388 (8)	0.42514 (8)	0.0419 (4)
H17A	0.4475	0.9953	0.4639	0.050*
C1B	0.70261 (11)	0.32146 (7)	0.29216 (7)	0.0309 (3)
C2B	0.71193 (12)	0.36314 (7)	0.24994 (8)	0.0336 (3)
H2BA	0.7182	0.4009	0.2636	0.040*
C3B	0.71234 (12)	0.35092 (7)	0.18666 (8)	0.0326 (3)
H3BA	0.7181	0.3803	0.1578	0.039*

C4B	0.70436 (11)	0.29630 (7)	0.16667 (7)	0.0287 (3)
H4BA	0.7045	0.2882	0.1238	0.034*
C5B	0.69594 (10)	0.25208 (7)	0.20877 (7)	0.0255 (3)
C6B	0.69224 (10)	0.19367 (7)	0.18988 (7)	0.0260 (3)
C7B	0.68425 (12)	0.15244 (7)	0.23553 (7)	0.0295 (3)
H7BA	0.6813	0.1139	0.2245	0.035*
C8B	0.68081 (11)	0.16813 (7)	0.29590 (7)	0.0298 (3)
H8BA	0.6747	0.1399	0.3261	0.036*
C9B	0.69409 (10)	0.26466 (7)	0.27264 (7)	0.0263 (3)
C10B	0.70130 (13)	0.33571 (8)	0.35973 (8)	0.0370 (4)
C11B	0.73397 (12)	0.11286 (7)	0.06376 (7)	0.0314 (3)
H11B	0.7411	0.1431	0.0362	0.038*
C12B	0.75329 (13)	0.05546 (7)	0.04440 (7)	0.0312 (3)
C13B	0.72313 (12)	0.00811 (7)	0.07544 (7)	0.0323 (3)
H13B	0.6866	0.0128	0.1100	0.039*
C14B	0.74556 (13)	−0.04518 (7)	0.05668 (8)	0.0349 (3)
H14B	0.7228	−0.0770	0.0773	0.042*
C15B	0.80194 (15)	−0.05220 (8)	0.00714 (9)	0.0414 (4)
C16B	0.83228 (18)	−0.00535 (9)	−0.02404 (10)	0.0491 (5)
H16B	0.8705	−0.0100	−0.0578	0.059*
C17B	0.80718 (16)	0.04761 (8)	−0.00628 (8)	0.0416 (4)
H17B	0.8266	0.0792	−0.0286	0.050*
C1C	0.45406 (12)	0.39089 (7)	0.19689 (8)	0.0331 (3)
C2C	0.46737 (13)	0.40745 (7)	0.13768 (9)	0.0378 (4)
H2CA	0.4726	0.4462	0.1287	0.045*
C3C	0.47331 (14)	0.36817 (8)	0.09071 (8)	0.0387 (4)
H3CA	0.4841	0.3803	0.0504	0.046*
C4C	0.46365 (13)	0.31206 (7)	0.10262 (8)	0.0339 (3)
H4CA	0.4663	0.2856	0.0701	0.041*
C5C	0.44977 (11)	0.29300 (7)	0.16300 (7)	0.0277 (3)
C6C	0.44602 (11)	0.23400 (7)	0.17822 (7)	0.0272 (3)
C7C	0.44761 (11)	0.21926 (7)	0.24094 (7)	0.0280 (3)
H7CA	0.4531	0.1810	0.2532	0.034*
C8C	0.44122 (11)	0.26022 (7)	0.28428 (7)	0.0284 (3)
H8CA	0.4387	0.2495	0.3262	0.034*
C9C	0.44641 (11)	0.33293 (7)	0.21064 (7)	0.0282 (3)
C10C	0.45138 (14)	0.43391 (7)	0.24691 (10)	0.0388 (4)
C11C	0.44711 (13)	0.10421 (7)	0.10625 (8)	0.0338 (3)
H11C	0.4270	0.1174	0.0654	0.041*
C12C	0.46553 (12)	0.04426 (7)	0.11611 (8)	0.0329 (3)
C13C	0.50844 (14)	0.02223 (8)	0.17285 (8)	0.0368 (3)
H13C	0.5268	0.0467	0.2068	0.044*
C14C	0.52437 (15)	−0.03457 (8)	0.18002 (8)	0.0398 (4)
H14C	0.5533	−0.0489	0.2189	0.048*
C15C	0.49837 (13)	−0.07113 (7)	0.13077 (8)	0.0349 (3)
C16C	0.45736 (15)	−0.04976 (8)	0.07377 (9)	0.0435 (4)
H16C	0.4403	−0.0742	0.0396	0.052*
C17C	0.44146 (15)	0.00738 (8)	0.06702 (9)	0.0430 (4)
H17C	0.4135	0.0217	0.0279	0.052*

C1D	0.64734 (12)	0.58375 (7)	0.24630 (8)	0.0314 (3)
C2D	0.66576 (13)	0.55508 (7)	0.30099 (9)	0.0357 (3)
H2DA	0.6749	0.5156	0.3003	0.043*
C3D	0.67130 (13)	0.58297 (7)	0.35787 (8)	0.0350 (3)
H3DA	0.6815	0.5623	0.3955	0.042*
C4D	0.66203 (12)	0.64020 (7)	0.35952 (7)	0.0297 (3)
H4DA	0.6683	0.6590	0.3983	0.036*
C5D	0.64323 (11)	0.67139 (6)	0.30411 (7)	0.0264 (3)
C6D	0.63804 (11)	0.73205 (6)	0.30392 (7)	0.0261 (3)
C7D	0.61317 (11)	0.75954 (7)	0.24666 (7)	0.0290 (3)
H7DA	0.6078	0.7992	0.2451	0.035*
C8D	0.59695 (12)	0.72870 (7)	0.19352 (7)	0.0310 (3)
H8DA	0.5786	0.7476	0.1554	0.037*
C9D	0.63124 (11)	0.64288 (6)	0.24669 (7)	0.0273 (3)
C10D	0.65298 (14)	0.55395 (8)	0.18568 (9)	0.0384 (4)
C11D	0.67856 (12)	0.84395 (7)	0.40515 (7)	0.0306 (3)
H11D	0.6895	0.8233	0.4428	0.037*
C12D	0.68713 (12)	0.90504 (7)	0.40613 (7)	0.0293 (3)
C13D	0.67608 (13)	0.93616 (7)	0.35097 (7)	0.0325 (3)
H13D	0.6591	0.9176	0.3125	0.039*
C14D	0.68964 (14)	0.99353 (7)	0.35203 (8)	0.0354 (3)
H14D	0.6826	1.0141	0.3143	0.042*
C15D	0.71355 (13)	1.02134 (7)	0.40816 (8)	0.0320 (3)
C16D	0.72377 (15)	0.99121 (7)	0.46336 (8)	0.0380 (4)
H16D	0.7396	1.0101	0.5018	0.046*
C17D	0.71078 (15)	0.93350 (7)	0.46207 (8)	0.0360 (3)
H17D	0.7181	0.9131	0.4999	0.043*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0433 (2)	0.02225 (17)	0.01919 (17)	−0.00186 (14)	0.00250 (13)	−0.00207 (12)
S2	0.0479 (2)	0.02552 (18)	0.01916 (16)	0.00029 (15)	0.00072 (14)	0.00022 (13)
F1A	0.0495 (6)	0.0568 (7)	0.0428 (6)	0.0014 (5)	0.0117 (5)	−0.0161 (5)
F2A	0.0412 (5)	0.0452 (6)	0.0479 (6)	0.0019 (5)	−0.0044 (4)	−0.0139 (5)
F3A	0.0801 (8)	0.0306 (5)	0.0525 (7)	−0.0039 (5)	0.0022 (6)	−0.0054 (5)
F1B	0.0497 (6)	0.0661 (8)	0.0330 (5)	0.0046 (6)	−0.0058 (4)	−0.0057 (5)
F2B	0.0466 (6)	0.0562 (7)	0.0360 (5)	−0.0044 (5)	0.0147 (4)	−0.0098 (5)
F3B	0.0756 (8)	0.0424 (6)	0.0409 (6)	−0.0103 (6)	0.0083 (5)	−0.0164 (5)
F1C	0.0541 (6)	0.0421 (6)	0.0510 (6)	0.0000 (5)	−0.0020 (5)	−0.0134 (5)
F2C	0.0470 (6)	0.0404 (6)	0.0672 (8)	−0.0005 (5)	0.0204 (5)	−0.0096 (5)
F3C	0.0721 (8)	0.0244 (5)	0.0706 (8)	−0.0046 (5)	0.0192 (6)	0.0002 (5)
F1D	0.0662 (7)	0.0610 (8)	0.0519 (7)	−0.0156 (6)	0.0271 (6)	−0.0221 (6)
F2D	0.0589 (6)	0.0400 (6)	0.0374 (5)	0.0005 (5)	−0.0047 (5)	−0.0104 (5)
F3D	0.0794 (8)	0.0325 (5)	0.0519 (7)	0.0123 (6)	0.0008 (6)	−0.0130 (5)
O1A	0.0510 (7)	0.0273 (6)	0.0309 (6)	−0.0041 (5)	−0.0018 (5)	0.0019 (5)
O1B	0.0842 (11)	0.0310 (7)	0.0724 (11)	0.0019 (7)	0.0401 (9)	−0.0066 (7)
O1C	0.0562 (8)	0.0296 (6)	0.0469 (7)	0.0001 (6)	0.0101 (6)	0.0015 (5)

O1D	0.0656 (8)	0.0214 (5)	0.0350 (6)	−0.0019 (5)	0.0162 (5)	−0.0015 (5)
O11	0.0501 (7)	0.0436 (7)	0.0273 (6)	0.0008 (6)	0.0064 (5)	0.0006 (5)
O12	0.0548 (7)	0.0327 (6)	0.0216 (5)	−0.0055 (5)	0.0032 (5)	0.0007 (4)
O13	0.0671 (8)	0.0250 (6)	0.0303 (6)	0.0039 (6)	0.0025 (5)	−0.0016 (5)
O14	0.0543 (7)	0.0307 (6)	0.0307 (6)	−0.0084 (5)	−0.0015 (5)	−0.0027 (5)
O21	0.0682 (8)	0.0303 (6)	0.0255 (5)	0.0011 (6)	−0.0020 (5)	0.0060 (5)
O22	0.0617 (8)	0.0409 (7)	0.0281 (6)	−0.0019 (6)	0.0061 (5)	0.0095 (5)
O23	0.0609 (8)	0.0509 (8)	0.0335 (6)	−0.0114 (7)	−0.0063 (6)	−0.0009 (6)
O24	0.0616 (8)	0.0462 (8)	0.0376 (7)	0.0118 (7)	−0.0007 (6)	−0.0127 (6)
O1W	0.0702 (9)	0.0519 (8)	0.0329 (7)	−0.0169 (8)	0.0026 (6)	0.0007 (6)
O2W	0.0613 (9)	0.0580 (9)	0.0371 (7)	0.0180 (7)	0.0129 (6)	−0.0039 (6)
O3W	0.0587 (10)	0.0836 (13)	0.0870 (14)	−0.0094 (10)	0.0159 (9)	−0.0483 (12)
O4W	0.0611 (10)	0.0841 (15)	0.1036 (17)	0.0200 (10)	0.0237 (10)	0.0408 (13)
N1A	0.0364 (6)	0.0333 (7)	0.0225 (6)	0.0004 (5)	0.0015 (5)	−0.0028 (5)
N2A	0.0369 (6)	0.0275 (6)	0.0243 (6)	−0.0019 (5)	0.0033 (5)	0.0022 (5)
N3A	0.0374 (6)	0.0266 (6)	0.0287 (6)	−0.0021 (5)	0.0033 (5)	0.0027 (5)
N1B	0.0334 (6)	0.0340 (7)	0.0200 (6)	0.0002 (5)	0.0041 (4)	−0.0001 (5)
N2B	0.0353 (6)	0.0252 (6)	0.0235 (6)	0.0008 (5)	0.0042 (5)	0.0018 (5)
N3B	0.0374 (7)	0.0258 (6)	0.0272 (6)	0.0016 (5)	0.0043 (5)	−0.0015 (5)
N1C	0.0332 (6)	0.0267 (6)	0.0288 (6)	0.0005 (5)	0.0045 (5)	−0.0029 (5)
N2C	0.0369 (6)	0.0273 (6)	0.0252 (6)	0.0021 (5)	0.0018 (5)	0.0004 (5)
N3C	0.0354 (6)	0.0272 (6)	0.0317 (7)	0.0021 (5)	0.0033 (5)	0.0008 (5)
N1D	0.0392 (7)	0.0290 (6)	0.0244 (6)	−0.0031 (5)	0.0045 (5)	−0.0024 (5)
N2D	0.0365 (6)	0.0207 (6)	0.0270 (6)	0.0003 (5)	0.0041 (5)	0.0007 (5)
N3D	0.0361 (6)	0.0200 (6)	0.0308 (6)	−0.0002 (5)	0.0042 (5)	0.0004 (5)
C1A	0.0326 (7)	0.0311 (8)	0.0328 (8)	0.0014 (6)	0.0063 (6)	−0.0015 (6)
C2A	0.0388 (8)	0.0294 (7)	0.0370 (8)	0.0022 (7)	0.0063 (6)	0.0043 (7)
C3A	0.0402 (8)	0.0359 (8)	0.0284 (7)	0.0018 (7)	0.0029 (6)	0.0064 (6)
C4A	0.0330 (7)	0.0338 (8)	0.0246 (7)	0.0010 (6)	0.0026 (5)	0.0003 (6)
C5A	0.0263 (6)	0.0295 (7)	0.0240 (7)	0.0005 (6)	0.0038 (5)	0.0006 (6)
C6A	0.0276 (7)	0.0304 (7)	0.0244 (7)	0.0005 (6)	0.0036 (5)	0.0014 (6)
C7A	0.0380 (8)	0.0301 (7)	0.0259 (7)	0.0012 (6)	0.0036 (6)	0.0029 (6)
C8A	0.0391 (8)	0.0373 (8)	0.0218 (7)	0.0024 (7)	0.0028 (5)	0.0037 (6)
C9A	0.0285 (7)	0.0316 (8)	0.0260 (7)	0.0021 (6)	0.0048 (5)	−0.0004 (6)
C10A	0.0399 (8)	0.0321 (8)	0.0389 (9)	0.0015 (7)	0.0059 (7)	−0.0047 (7)
C11A	0.0423 (8)	0.0315 (8)	0.0269 (7)	−0.0073 (7)	0.0029 (6)	0.0032 (6)
C12A	0.0379 (8)	0.0302 (8)	0.0280 (7)	−0.0058 (6)	0.0043 (6)	0.0003 (6)
C13A	0.0442 (8)	0.0315 (8)	0.0243 (7)	−0.0018 (7)	0.0027 (6)	−0.0022 (6)
C14A	0.0471 (9)	0.0327 (8)	0.0238 (7)	0.0030 (7)	0.0034 (6)	0.0031 (6)
C15A	0.0343 (7)	0.0265 (7)	0.0294 (7)	−0.0009 (6)	0.0032 (5)	0.0002 (6)
C16A	0.0585 (10)	0.0357 (9)	0.0241 (7)	−0.0109 (8)	0.0018 (7)	−0.0002 (6)
C17A	0.0632 (11)	0.0371 (9)	0.0246 (7)	−0.0122 (8)	0.0018 (7)	0.0043 (7)
C1B	0.0293 (7)	0.0346 (8)	0.0289 (8)	0.0007 (6)	0.0033 (5)	−0.0048 (6)
C2B	0.0340 (8)	0.0296 (7)	0.0375 (8)	−0.0007 (6)	0.0053 (6)	−0.0039 (6)
C3B	0.0329 (7)	0.0304 (8)	0.0348 (8)	0.0004 (6)	0.0052 (6)	0.0048 (6)
C4B	0.0294 (7)	0.0315 (7)	0.0256 (7)	−0.0001 (6)	0.0047 (5)	0.0010 (6)
C5B	0.0239 (6)	0.0287 (7)	0.0238 (7)	0.0008 (5)	0.0030 (5)	0.0008 (6)
C6B	0.0245 (6)	0.0285 (7)	0.0251 (7)	0.0021 (5)	0.0026 (5)	0.0008 (6)
C7B	0.0341 (7)	0.0273 (7)	0.0273 (7)	0.0004 (6)	0.0043 (5)	0.0026 (6)

C8B	0.0316 (7)	0.0316 (7)	0.0262 (7)	0.0019 (6)	0.0034 (5)	0.0065 (6)
C9B	0.0238 (6)	0.0308 (7)	0.0240 (7)	0.0006 (5)	0.0015 (5)	−0.0003 (6)
C10B	0.0403 (8)	0.0382 (9)	0.0323 (8)	−0.0021 (7)	0.0039 (6)	−0.0088 (7)
C11B	0.0406 (8)	0.0288 (7)	0.0246 (7)	−0.0009 (6)	0.0034 (6)	0.0014 (6)
C12B	0.0411 (8)	0.0283 (7)	0.0238 (7)	0.0001 (6)	0.0026 (6)	0.0008 (6)
C13B	0.0400 (8)	0.0328 (8)	0.0249 (7)	0.0023 (7)	0.0069 (6)	0.0037 (6)
C14B	0.0426 (8)	0.0305 (8)	0.0320 (8)	0.0009 (7)	0.0067 (6)	0.0045 (6)
C15B	0.0529 (10)	0.0298 (8)	0.0440 (9)	0.0010 (8)	0.0155 (8)	−0.0049 (7)
C16B	0.0717 (13)	0.0392 (10)	0.0419 (10)	−0.0042 (9)	0.0294 (9)	−0.0043 (8)
C17B	0.0637 (11)	0.0326 (8)	0.0313 (8)	−0.0057 (8)	0.0173 (8)	0.0007 (7)
C1C	0.0301 (7)	0.0285 (8)	0.0404 (9)	−0.0013 (6)	0.0024 (6)	0.0026 (7)
C2C	0.0395 (8)	0.0297 (8)	0.0434 (9)	−0.0041 (7)	0.0012 (7)	0.0088 (7)
C3C	0.0422 (9)	0.0405 (9)	0.0330 (8)	−0.0029 (7)	0.0028 (6)	0.0105 (7)
C4C	0.0384 (8)	0.0347 (8)	0.0284 (7)	−0.0005 (7)	0.0030 (6)	0.0024 (6)
C5C	0.0255 (6)	0.0282 (7)	0.0288 (7)	0.0000 (6)	0.0013 (5)	0.0019 (6)
C6C	0.0248 (6)	0.0282 (7)	0.0284 (7)	0.0012 (5)	0.0030 (5)	0.0007 (6)
C7C	0.0300 (7)	0.0255 (7)	0.0283 (7)	−0.0011 (6)	0.0030 (5)	0.0014 (6)
C8C	0.0292 (7)	0.0301 (7)	0.0261 (7)	−0.0015 (6)	0.0039 (5)	0.0022 (6)
C9C	0.0261 (6)	0.0275 (7)	0.0307 (7)	0.0008 (6)	0.0028 (5)	0.0016 (6)
C10C	0.0404 (9)	0.0254 (7)	0.0516 (10)	−0.0023 (7)	0.0095 (7)	0.0002 (7)
C11C	0.0415 (8)	0.0319 (8)	0.0272 (7)	0.0038 (7)	0.0007 (6)	−0.0019 (6)
C12C	0.0379 (8)	0.0308 (8)	0.0298 (8)	0.0027 (6)	0.0030 (6)	−0.0036 (6)
C13C	0.0486 (9)	0.0344 (8)	0.0274 (7)	0.0004 (7)	0.0049 (6)	−0.0041 (6)
C14C	0.0523 (10)	0.0374 (9)	0.0297 (8)	0.0039 (8)	0.0043 (7)	0.0025 (7)
C15C	0.0375 (8)	0.0299 (8)	0.0386 (8)	−0.0002 (7)	0.0105 (6)	−0.0004 (7)
C16C	0.0522 (10)	0.0344 (9)	0.0414 (9)	0.0016 (8)	−0.0046 (7)	−0.0109 (8)
C17C	0.0575 (10)	0.0373 (9)	0.0315 (8)	0.0082 (8)	−0.0066 (7)	−0.0047 (7)
C1D	0.0349 (7)	0.0265 (7)	0.0326 (8)	−0.0029 (6)	0.0035 (6)	−0.0045 (6)
C2D	0.0421 (8)	0.0215 (7)	0.0423 (9)	−0.0004 (6)	−0.0003 (7)	−0.0015 (7)
C3D	0.0447 (8)	0.0267 (8)	0.0323 (8)	−0.0007 (7)	−0.0003 (6)	0.0050 (6)
C4D	0.0357 (7)	0.0261 (7)	0.0270 (7)	−0.0016 (6)	0.0027 (5)	−0.0004 (6)
C5D	0.0273 (6)	0.0246 (7)	0.0275 (7)	−0.0020 (6)	0.0047 (5)	−0.0008 (6)
C6D	0.0264 (6)	0.0244 (7)	0.0281 (7)	−0.0014 (5)	0.0054 (5)	−0.0002 (6)
C7D	0.0331 (7)	0.0240 (7)	0.0299 (7)	0.0000 (6)	0.0039 (5)	0.0031 (6)
C8D	0.0361 (7)	0.0310 (8)	0.0259 (7)	−0.0007 (6)	0.0043 (5)	0.0039 (6)
C9D	0.0287 (7)	0.0253 (7)	0.0282 (7)	−0.0031 (6)	0.0042 (5)	−0.0012 (6)
C10D	0.0473 (9)	0.0297 (8)	0.0381 (9)	−0.0012 (7)	0.0052 (7)	−0.0086 (7)
C11D	0.0412 (8)	0.0231 (7)	0.0282 (7)	0.0018 (6)	0.0067 (6)	0.0020 (6)
C12D	0.0381 (7)	0.0221 (7)	0.0282 (7)	0.0016 (6)	0.0060 (6)	−0.0008 (6)
C13D	0.0476 (9)	0.0250 (7)	0.0251 (7)	0.0030 (6)	0.0043 (6)	−0.0019 (6)
C14D	0.0544 (9)	0.0247 (7)	0.0280 (7)	0.0043 (7)	0.0096 (6)	0.0034 (6)
C15D	0.0415 (8)	0.0224 (7)	0.0339 (8)	0.0023 (6)	0.0120 (6)	−0.0005 (6)
C16D	0.0606 (10)	0.0267 (8)	0.0268 (7)	−0.0016 (7)	0.0055 (7)	−0.0047 (6)
C17D	0.0560 (10)	0.0269 (8)	0.0248 (7)	0.0002 (7)	0.0034 (6)	0.0025 (6)

Geometric parameters (Å, °)

S1—O12	1.4750 (11)	C14A—H14A	0.9500
S1—O11	1.4767 (13)	C15A—C16A	1.384 (2)

S1—O14	1.4782 (13)	C16A—C17A	1.387 (3)
S1—O13	1.4808 (13)	C16A—H16A	0.9500
S2—O24	1.4636 (14)	C17A—H17A	0.9500
S2—O23	1.4786 (15)	C1B—C2B	1.369 (2)
S2—O21	1.4794 (13)	C1B—C9B	1.420 (2)
S2—O22	1.4838 (13)	C1B—C10B	1.509 (2)
F1A—C10A	1.338 (2)	C2B—C3B	1.405 (2)
F2A—C10A	1.345 (2)	C2B—H2BA	0.9500
F3A—C10A	1.326 (2)	C3B—C4B	1.374 (2)
F1B—C10B	1.339 (2)	C3B—H3BA	0.9500
F2B—C10B	1.337 (2)	C4B—C5B	1.410 (2)
F3B—C10B	1.337 (2)	C4B—H4BA	0.9500
F1C—C10C	1.343 (2)	C5B—C9B	1.422 (2)
F2C—C10C	1.337 (2)	C5B—C6B	1.452 (2)
F3C—C10C	1.329 (2)	C6B—C7B	1.410 (2)
F1D—C10D	1.335 (2)	C7B—C8B	1.370 (2)
F2D—C10D	1.332 (2)	C7B—H7BA	0.9500
F3D—C10D	1.337 (2)	C8B—H8BA	0.9500
O1A—C15A	1.357 (2)	C11B—C12B	1.465 (2)
O1A—H1A	0.8400	C11B—H11B	0.9500
O1B—C15B	1.355 (2)	C12B—C13B	1.400 (2)
O1B—H1B	0.8400	C12B—C17B	1.400 (2)
O1C—C15C	1.357 (2)	C13B—C14B	1.379 (2)
O1C—H1C	0.8400	C13B—H13B	0.9500
O1D—C15D	1.3564 (19)	C14B—C15B	1.398 (2)
O1D—H1D	0.8400	C14B—H14B	0.9500
O1W—H1W1	0.810 (17)	C15B—C16B	1.393 (3)
O1W—H1W2	0.812 (17)	C16B—C17B	1.375 (3)
O2W—H2W1	0.821 (17)	C16B—H16B	0.9500
O2W—H2W2	0.828 (17)	C17B—H17B	0.9500
O3W—H3W1	0.824 (18)	C1C—C2C	1.377 (3)
O3W—H3W2	0.841 (18)	C1C—C9C	1.421 (2)
O4W—H4W1	0.835 (18)	C1C—C10C	1.498 (3)
O4W—H4W2	0.820 (19)	C2C—C3C	1.395 (3)
N1A—C8A	1.343 (2)	C2C—H2CA	0.9500
N1A—C9A	1.381 (2)	C3C—C4C	1.373 (3)
N1A—H1AA	0.8800	C3C—H3CA	0.9500
N2A—C6A	1.329 (2)	C4C—C5C	1.421 (2)
N2A—N3A	1.3870 (19)	C4C—H4CA	0.9500
N2A—H2AB	0.8800	C5C—C9C	1.411 (2)
N3A—C11A	1.271 (2)	C5C—C6C	1.448 (2)
N1B—C8B	1.340 (2)	C6C—C7C	1.405 (2)
N1B—C9B	1.372 (2)	C7C—C8C	1.367 (2)
N1B—H1BA	0.8800	C7C—H7CA	0.9500
N2B—C6B	1.335 (2)	C8C—H8CA	0.9500
N2B—N3B	1.3938 (18)	C11C—C12C	1.463 (2)
N2B—H2BB	0.8800	C11C—H11C	0.9500
N3B—C11B	1.276 (2)	C12C—C17C	1.390 (2)
N1C—C8C	1.342 (2)	C12C—C13C	1.399 (2)

N1C—C9C	1.376 (2)	C13C—C14C	1.378 (3)
N1C—H1CA	0.8800	C13C—H13C	0.9500
N2C—C6C	1.337 (2)	C14C—C15C	1.392 (3)
N2C—N3C	1.3898 (19)	C14C—H14C	0.9500
N2C—H2CB	0.8800	C15C—C16C	1.390 (3)
N3C—C11C	1.278 (2)	C16C—C17C	1.385 (3)
N1D—C8D	1.347 (2)	C16C—H16C	0.9500
N1D—C9D	1.371 (2)	C17C—H17C	0.9500
N1D—H1DA	0.8800	C1D—C2D	1.367 (3)
N2D—C6D	1.337 (2)	C1D—C9D	1.428 (2)
N2D—N3D	1.3859 (17)	C1D—C10D	1.506 (2)
N2D—H2DB	0.8800	C2D—C3D	1.397 (3)
N3D—C11D	1.271 (2)	C2D—H2DA	0.9500
C1A—C2A	1.375 (2)	C3D—C4D	1.372 (2)
C1A—C9A	1.416 (2)	C3D—H3DA	0.9500
C1A—C10A	1.497 (2)	C4D—C5D	1.412 (2)
C2A—C3A	1.402 (3)	C4D—H4DA	0.9500
C2A—H2AA	0.9500	C5D—C9D	1.413 (2)
C3A—C4A	1.366 (2)	C5D—C6D	1.449 (2)
C3A—H3AA	0.9500	C6D—C7D	1.410 (2)
C4A—C5A	1.416 (2)	C7D—C8D	1.364 (2)
C4A—H4AA	0.9500	C7D—H7DA	0.9500
C5A—C9A	1.409 (2)	C8D—H8DA	0.9500
C5A—C6A	1.446 (2)	C11D—C12D	1.462 (2)
C6A—C7A	1.410 (2)	C11D—H11D	0.9500
C7A—C8A	1.363 (2)	C12D—C17D	1.395 (2)
C7A—H7AA	0.9500	C12D—C13D	1.402 (2)
C8A—H8AA	0.9500	C13D—C14D	1.381 (2)
C11A—C12A	1.458 (2)	C13D—H13D	0.9500
C11A—H11A	0.9500	C14D—C15D	1.392 (2)
C12A—C17A	1.390 (2)	C14D—H14D	0.9500
C12A—C13A	1.395 (2)	C15D—C16D	1.390 (2)
C13A—C14A	1.379 (2)	C16D—C17D	1.388 (2)
C13A—H13A	0.9500	C16D—H16D	0.9500
C14A—C15A	1.398 (2)	C17D—H17D	0.9500
O12—S1—O11	108.99 (8)	F3B—C10B—C1B	112.13 (16)
O12—S1—O14	110.19 (7)	F2B—C10B—C1B	111.89 (14)
O11—S1—O14	110.05 (8)	F1B—C10B—C1B	112.10 (15)
O12—S1—O13	109.70 (7)	N3B—C11B—C12B	120.67 (15)
O11—S1—O13	108.58 (8)	N3B—C11B—H11B	119.7
O14—S1—O13	109.30 (8)	C12B—C11B—H11B	119.7
O24—S2—O23	110.16 (9)	C13B—C12B—C17B	118.49 (16)
O24—S2—O21	110.23 (8)	C13B—C12B—C11B	123.02 (15)
O23—S2—O21	109.45 (9)	C17B—C12B—C11B	118.46 (15)
O24—S2—O22	109.52 (9)	C14B—C13B—C12B	121.04 (15)
O23—S2—O22	109.39 (8)	C14B—C13B—H13B	119.5
O21—S2—O22	108.07 (8)	C12B—C13B—H13B	119.5
C15A—O1A—H1A	109.5	C13B—C14B—C15B	119.69 (16)
C15B—O1B—H1B	109.5	C13B—C14B—H14B	120.2

C15C—O1C—H1C	109.5	C15B—C14B—H14B	120.2
C15D—O1D—H1D	109.5	O1B—C15B—C16B	118.08 (17)
H1W1—O1W—H1W2	109 (3)	O1B—C15B—C14B	122.24 (18)
H2W1—O2W—H2W2	103 (2)	C16B—C15B—C14B	119.67 (17)
H3W1—O3W—H3W2	104 (3)	C17B—C16B—C15B	120.35 (16)
H4W1—O4W—H4W2	104 (3)	C17B—C16B—H16B	119.8
C8A—N1A—C9A	121.06 (14)	C15B—C16B—H16B	119.8
C8A—N1A—H1AA	119.5	C16B—C17B—C12B	120.71 (17)
C9A—N1A—H1AA	119.5	C16B—C17B—H17B	119.6
C6A—N2A—N3A	118.18 (13)	C12B—C17B—H17B	119.6
C6A—N2A—H2AB	120.9	C2C—C1C—C9C	119.74 (16)
N3A—N2A—H2AB	120.9	C2C—C1C—C10C	119.85 (16)
C11A—N3A—N2A	114.69 (13)	C9C—C1C—C10C	120.38 (16)
C8B—N1B—C9B	121.76 (13)	C1C—C2C—C3C	121.03 (16)
C8B—N1B—H1BA	119.1	C1C—C2C—H2CA	119.5
C9B—N1B—H1BA	119.1	C3C—C2C—H2CA	119.5
C6B—N2B—N3B	118.13 (13)	C4C—C3C—C2C	120.17 (16)
C6B—N2B—H2BB	120.9	C4C—C3C—H3CA	119.9
N3B—N2B—H2BB	120.9	C2C—C3C—H3CA	119.9
C11B—N3B—N2B	114.36 (14)	C3C—C4C—C5C	120.78 (16)
C8C—N1C—C9C	121.06 (14)	C3C—C4C—H4CA	119.6
C8C—N1C—H1CA	119.5	C5C—C4C—H4CA	119.6
C9C—N1C—H1CA	119.5	C9C—C5C—C4C	118.67 (15)
C6C—N2C—N3C	118.65 (13)	C9C—C5C—C6C	118.94 (14)
C6C—N2C—H2CB	120.7	C4C—C5C—C6C	122.24 (15)
N3C—N2C—H2CB	120.7	N2C—C6C—C7C	121.53 (14)
C11C—N3C—N2C	115.06 (14)	N2C—C6C—C5C	120.55 (14)
C8D—N1D—C9D	121.28 (14)	C7C—C6C—C5C	117.90 (14)
C8D—N1D—H1DA	119.4	C8C—C7C—C6C	119.59 (14)
C9D—N1D—H1DA	119.4	C8C—C7C—H7CA	120.2
C6D—N2D—N3D	117.71 (13)	C6C—C7C—H7CA	120.2
C6D—N2D—H2DB	121.1	N1C—C8C—C7C	122.68 (14)
N3D—N2D—H2DB	121.1	N1C—C8C—H8CA	118.7
C11D—N3D—N2D	115.80 (13)	C7C—C8C—H8CA	118.7
C2A—C1A—C9A	120.45 (15)	N1C—C9C—C5C	119.35 (14)
C2A—C1A—C10A	119.84 (16)	N1C—C9C—C1C	121.05 (15)
C9A—C1A—C10A	119.70 (15)	C5C—C9C—C1C	119.57 (15)
C1A—C2A—C3A	120.19 (16)	F3C—C10C—F2C	107.13 (15)
C1A—C2A—H2AA	119.9	F3C—C10C—F1C	106.28 (15)
C3A—C2A—H2AA	119.9	F2C—C10C—F1C	105.80 (16)
C4A—C3A—C2A	120.50 (15)	F3C—C10C—C1C	112.48 (16)
C4A—C3A—H3AA	119.8	F2C—C10C—C1C	112.50 (15)
C2A—C3A—H3AA	119.8	F1C—C10C—C1C	112.18 (15)
C3A—C4A—C5A	120.54 (15)	N3C—C11C—C12C	121.87 (15)
C3A—C4A—H4AA	119.7	N3C—C11C—H11C	119.1
C5A—C4A—H4AA	119.7	C12C—C11C—H11C	119.1
C9A—C5A—C4A	119.19 (15)	C17C—C12C—C13C	118.11 (17)
C9A—C5A—C6A	118.83 (14)	C17C—C12C—C11C	119.13 (16)
C4A—C5A—C6A	121.98 (14)	C13C—C12C—C11C	122.75 (15)

N2A—C6A—C7A	121.25 (15)	C14C—C13C—C12C	120.75 (16)
N2A—C6A—C5A	120.74 (14)	C14C—C13C—H13C	119.6
C7A—C6A—C5A	118.01 (14)	C12C—C13C—H13C	119.6
C8A—C7A—C6A	119.85 (15)	C13C—C14C—C15C	120.54 (17)
C8A—C7A—H7AA	120.1	C13C—C14C—H14C	119.7
C6A—C7A—H7AA	120.1	C15C—C14C—H14C	119.7
N1A—C8A—C7A	122.55 (15)	O1C—C15C—C16C	122.71 (17)
N1A—C8A—H8AA	118.7	O1C—C15C—C14C	117.90 (17)
C7A—C8A—H8AA	118.7	C16C—C15C—C14C	119.39 (17)
N1A—C9A—C5A	119.55 (15)	C17C—C16C—C15C	119.66 (17)
N1A—C9A—C1A	121.49 (15)	C17C—C16C—H16C	120.2
C5A—C9A—C1A	118.96 (14)	C15C—C16C—H16C	120.2
F3A—C10A—F1A	107.99 (15)	C16C—C17C—C12C	121.54 (17)
F3A—C10A—F2A	106.30 (15)	C16C—C17C—H17C	119.2
F1A—C10A—F2A	106.34 (15)	C12C—C17C—H17C	119.2
F3A—C10A—C1A	112.91 (15)	C2D—C1D—C9D	120.07 (15)
F1A—C10A—C1A	112.11 (15)	C2D—C1D—C10D	120.03 (15)
F2A—C10A—C1A	110.80 (14)	C9D—C1D—C10D	119.68 (15)
N3A—C11A—C12A	121.08 (15)	C1D—C2D—C3D	120.98 (15)
N3A—C11A—H11A	119.5	C1D—C2D—H2DA	119.5
C12A—C11A—H11A	119.5	C3D—C2D—H2DA	119.5
C17A—C12A—C13A	118.46 (16)	C4D—C3D—C2D	120.11 (15)
C17A—C12A—C11A	118.37 (15)	C4D—C3D—H3DA	119.9
C13A—C12A—C11A	123.12 (15)	C2D—C3D—H3DA	119.9
C14A—C13A—C12A	120.05 (15)	C3D—C4D—C5D	120.67 (15)
C14A—C13A—H13A	120.0	C3D—C4D—H4DA	119.7
C12A—C13A—H13A	120.0	C5D—C4D—H4DA	119.7
C13A—C14A—C15A	120.76 (15)	C4D—C5D—C9D	119.23 (14)
C13A—C14A—H14A	119.6	C4D—C5D—C6D	122.20 (14)
C15A—C14A—H14A	119.6	C9D—C5D—C6D	118.56 (14)
O1A—C15A—C16A	122.69 (15)	N2D—C6D—C7D	121.76 (14)
O1A—C15A—C14A	117.67 (14)	N2D—C6D—C5D	119.98 (14)
C16A—C15A—C14A	119.61 (16)	C7D—C6D—C5D	118.25 (14)
C15A—C16A—C17A	119.03 (16)	C8D—C7D—C6D	119.49 (15)
C15A—C16A—H16A	120.5	C8D—C7D—H7DA	120.3
C17A—C16A—H16A	120.5	C6D—C7D—H7DA	120.3
C16A—C17A—C12A	121.83 (16)	N1D—C8D—C7D	122.62 (15)
C16A—C17A—H17A	119.1	N1D—C8D—H8DA	118.7
C12A—C17A—H17A	119.1	C7D—C8D—H8DA	118.7
C2B—C1B—C9B	120.26 (15)	N1D—C9D—C5D	119.54 (14)
C2B—C1B—C10B	120.03 (16)	N1D—C9D—C1D	121.78 (14)
C9B—C1B—C10B	119.71 (15)	C5D—C9D—C1D	118.67 (14)
C1B—C2B—C3B	121.04 (16)	F2D—C10D—F1D	106.48 (16)
C1B—C2B—H2BA	119.5	F2D—C10D—F3D	106.44 (15)
C3B—C2B—H2BA	119.5	F1D—C10D—F3D	107.05 (16)
C4B—C3B—C2B	119.78 (15)	F2D—C10D—C1D	113.44 (15)
C4B—C3B—H3BA	120.1	F1D—C10D—C1D	111.08 (14)
C2B—C3B—H3BA	120.1	F3D—C10D—C1D	111.95 (16)
C3B—C4B—C5B	120.95 (14)	N3D—C11D—C12D	119.94 (14)

C3B—C4B—H4BA	119.5	N3D—C11D—H11D	120.0
C5B—C4B—H4BA	119.5	C12D—C11D—H11D	120.0
C4B—C5B—C9B	119.12 (14)	C17D—C12D—C13D	118.45 (15)
C4B—C5B—C6B	122.54 (14)	C17D—C12D—C11D	120.48 (14)
C9B—C5B—C6B	118.31 (14)	C13D—C12D—C11D	121.02 (14)
N2B—C6B—C7B	120.89 (14)	C14D—C13D—C12D	120.69 (15)
N2B—C6B—C5B	120.79 (14)	C14D—C13D—H13D	119.7
C7B—C6B—C5B	118.29 (14)	C12D—C13D—H13D	119.7
C8B—C7B—C6B	119.77 (15)	C13D—C14D—C15D	120.25 (15)
C8B—C7B—H7BA	120.1	C13D—C14D—H14D	119.9
C6B—C7B—H7BA	120.1	C15D—C14D—H14D	119.9
N1B—C8B—C7B	122.33 (15)	O1D—C15D—C16D	122.39 (15)
N1B—C8B—H8BA	118.8	O1D—C15D—C14D	117.78 (15)
C7B—C8B—H8BA	118.8	C16D—C15D—C14D	119.82 (15)
N1B—C9B—C1B	121.65 (14)	C17D—C16D—C15D	119.76 (16)
N1B—C9B—C5B	119.50 (14)	C17D—C16D—H16D	120.1
C1B—C9B—C5B	118.84 (14)	C15D—C16D—H16D	120.1
F3B—C10B—F2B	107.05 (15)	C16D—C17D—C12D	121.03 (15)
F3B—C10B—F1B	107.03 (15)	C16D—C17D—H17D	119.5
F2B—C10B—F1B	106.26 (16)	C12D—C17D—H17D	119.5
C6A—N2A—N3A—C11A	174.68 (15)	C13B—C12B—C17B—C16B	−1.8 (3)
C6B—N2B—N3B—C11B	−166.53 (14)	C11B—C12B—C17B—C16B	176.22 (19)
C6C—N2C—N3C—C11C	175.23 (15)	C9C—C1C—C2C—C3C	0.1 (3)
C6D—N2D—N3D—C11D	−177.70 (14)	C10C—C1C—C2C—C3C	177.96 (16)
C9A—C1A—C2A—C3A	2.4 (2)	C1C—C2C—C3C—C4C	1.5 (3)
C10A—C1A—C2A—C3A	−176.03 (16)	C2C—C3C—C4C—C5C	−1.4 (3)
C1A—C2A—C3A—C4A	1.4 (3)	C3C—C4C—C5C—C9C	−0.2 (2)
C2A—C3A—C4A—C5A	−3.0 (2)	C3C—C4C—C5C—C6C	−175.78 (15)
C3A—C4A—C5A—C9A	0.7 (2)	N3C—N2C—C6C—C7C	−8.9 (2)
C3A—C4A—C5A—C6A	−178.49 (15)	N3C—N2C—C6C—C5C	169.30 (13)
N3A—N2A—C6A—C7A	−3.0 (2)	C9C—C5C—C6C—N2C	176.53 (14)
N3A—N2A—C6A—C5A	177.14 (13)	C4C—C5C—C6C—N2C	−7.9 (2)
C9A—C5A—C6A—N2A	175.32 (13)	C9C—C5C—C6C—C7C	−5.2 (2)
C4A—C5A—C6A—N2A	−5.5 (2)	C4C—C5C—C6C—C7C	170.37 (14)
C9A—C5A—C6A—C7A	−4.6 (2)	N2C—C6C—C7C—C8C	−174.45 (14)
C4A—C5A—C6A—C7A	174.61 (14)	C5C—C6C—C7C—C8C	7.3 (2)
N2A—C6A—C7A—C8A	−176.70 (15)	C9C—N1C—C8C—C7C	−2.9 (2)
C5A—C6A—C7A—C8A	3.2 (2)	C6C—C7C—C8C—N1C	−3.4 (2)
C9A—N1A—C8A—C7A	−2.0 (2)	C8C—N1C—C9C—C5C	5.0 (2)
C6A—C7A—C8A—N1A	0.1 (3)	C8C—N1C—C9C—C1C	−173.31 (14)
C8A—N1A—C9A—C5A	0.5 (2)	C4C—C5C—C9C—N1C	−176.54 (14)
C8A—N1A—C9A—C1A	−178.97 (15)	C6C—C5C—C9C—N1C	−0.8 (2)
C4A—C5A—C9A—N1A	−176.41 (13)	C4C—C5C—C9C—C1C	1.8 (2)
C6A—C5A—C9A—N1A	2.8 (2)	C6C—C5C—C9C—C1C	177.50 (13)
C4A—C5A—C9A—C1A	3.1 (2)	C2C—C1C—C9C—N1C	176.53 (15)
C6A—C5A—C9A—C1A	−177.73 (13)	C10C—C1C—C9C—N1C	−1.3 (2)
C2A—C1A—C9A—N1A	174.83 (15)	C2C—C1C—C9C—C5C	−1.7 (2)
C10A—C1A—C9A—N1A	−6.7 (2)	C10C—C1C—C9C—C5C	−179.57 (15)
C2A—C1A—C9A—C5A	−4.6 (2)	C2C—C1C—C10C—F3C	−1.2 (2)

C10A—C1A—C9A—C5A	173.83 (14)	C9C—C1C—C10C—F3C	176.61 (15)
C2A—C1A—C10A—F3A	7.6 (2)	C2C—C1C—C10C—F2C	119.88 (18)
C9A—C1A—C10A—F3A	−170.92 (15)	C9C—C1C—C10C—F2C	−62.3 (2)
C2A—C1A—C10A—F1A	−114.69 (18)	C2C—C1C—C10C—F1C	−120.97 (18)
C9A—C1A—C10A—F1A	66.8 (2)	C9C—C1C—C10C—F1C	56.9 (2)
C2A—C1A—C10A—F2A	126.68 (17)	N2C—N3C—C11C—C12C	175.75 (14)
C9A—C1A—C10A—F2A	−51.8 (2)	N3C—C11C—C12C—C17C	172.15 (17)
N2A—N3A—C11A—C12A	178.14 (14)	N3C—C11C—C12C—C13C	−9.1 (3)
N3A—C11A—C12A—C17A	−171.37 (17)	C17C—C12C—C13C—C14C	−1.3 (3)
N3A—C11A—C12A—C13A	6.0 (3)	C11C—C12C—C13C—C14C	179.97 (17)
C17A—C12A—C13A—C14A	3.8 (3)	C12C—C13C—C14C—C15C	0.3 (3)
C11A—C12A—C13A—C14A	−173.53 (17)	C13C—C14C—C15C—O1C	−179.77 (16)
C12A—C13A—C14A—C15A	0.7 (3)	C13C—C14C—C15C—C16C	0.9 (3)
C13A—C14A—C15A—O1A	177.59 (16)	O1C—C15C—C16C—C17C	179.70 (18)
C13A—C14A—C15A—C16A	−4.1 (3)	C14C—C15C—C16C—C17C	−1.0 (3)
O1A—C15A—C16A—C17A	−179.04 (17)	C15C—C16C—C17C—C12C	0.0 (3)
C14A—C15A—C16A—C17A	2.7 (3)	C13C—C12C—C17C—C16C	1.2 (3)
C15A—C16A—C17A—C12A	1.9 (3)	C11C—C12C—C17C—C16C	179.97 (18)
C13A—C12A—C17A—C16A	−5.2 (3)	C9D—C1D—C2D—C3D	−1.4 (3)
C11A—C12A—C17A—C16A	172.26 (18)	C10D—C1D—C2D—C3D	173.24 (16)
C9B—C1B—C2B—C3B	0.6 (2)	C1D—C2D—C3D—C4D	−2.5 (3)
C10B—C1B—C2B—C3B	−179.37 (15)	C2D—C3D—C4D—C5D	2.3 (3)
C1B—C2B—C3B—C4B	−0.7 (2)	C3D—C4D—C5D—C9D	1.7 (2)
C2B—C3B—C4B—C5B	−0.1 (2)	C3D—C4D—C5D—C6D	−176.80 (15)
C3B—C4B—C5B—C9B	1.0 (2)	N3D—N2D—C6D—C7D	−2.7 (2)
C3B—C4B—C5B—C6B	−176.94 (14)	N3D—N2D—C6D—C5D	176.75 (12)
N3B—N2B—C6B—C7B	−5.8 (2)	C4D—C5D—C6D—N2D	4.2 (2)
N3B—N2B—C6B—C5B	172.22 (13)	C9D—C5D—C6D—N2D	−174.39 (13)
C4B—C5B—C6B—N2B	1.6 (2)	C4D—C5D—C6D—C7D	−176.38 (14)
C9B—C5B—C6B—N2B	−176.40 (13)	C9D—C5D—C6D—C7D	5.1 (2)
C4B—C5B—C6B—C7B	179.70 (14)	N2D—C6D—C7D—C8D	178.09 (14)
C9B—C5B—C6B—C7B	1.7 (2)	C5D—C6D—C7D—C8D	−1.4 (2)
N2B—C6B—C7B—C8B	177.71 (14)	C9D—N1D—C8D—C7D	0.7 (2)
C5B—C6B—C7B—C8B	−0.4 (2)	C6D—C7D—C8D—N1D	−1.6 (2)
C9B—N1B—C8B—C7B	0.4 (2)	C8D—N1D—C9D—C5D	3.2 (2)
C6B—C7B—C8B—N1B	−0.7 (2)	C8D—N1D—C9D—C1D	−175.89 (14)
C8B—N1B—C9B—C1B	−177.93 (14)	C4D—C5D—C9D—N1D	175.41 (14)
C8B—N1B—C9B—C5B	1.0 (2)	C6D—C5D—C9D—N1D	−6.0 (2)
C2B—C1B—C9B—N1B	179.26 (14)	C4D—C5D—C9D—C1D	−5.5 (2)
C10B—C1B—C9B—N1B	−0.8 (2)	C6D—C5D—C9D—C1D	173.12 (13)
C2B—C1B—C9B—C5B	0.3 (2)	C2D—C1D—C9D—N1D	−175.57 (15)
C10B—C1B—C9B—C5B	−179.72 (14)	C10D—C1D—C9D—N1D	9.8 (2)
C4B—C5B—C9B—N1B	179.91 (13)	C2D—C1D—C9D—C5D	5.3 (2)
C6B—C5B—C9B—N1B	−2.0 (2)	C10D—C1D—C9D—C5D	−169.30 (14)
C4B—C5B—C9B—C1B	−1.1 (2)	C2D—C1D—C10D—F2D	122.03 (18)
C6B—C5B—C9B—C1B	176.96 (13)	C9D—C1D—C10D—F2D	−63.3 (2)
C2B—C1B—C10B—F3B	−1.7 (2)	C2D—C1D—C10D—F1D	−118.07 (19)
C9B—C1B—C10B—F3B	178.35 (14)	C9D—C1D—C10D—F1D	56.6 (2)
C2B—C1B—C10B—F2B	118.63 (18)	C2D—C1D—C10D—F3D	1.5 (2)

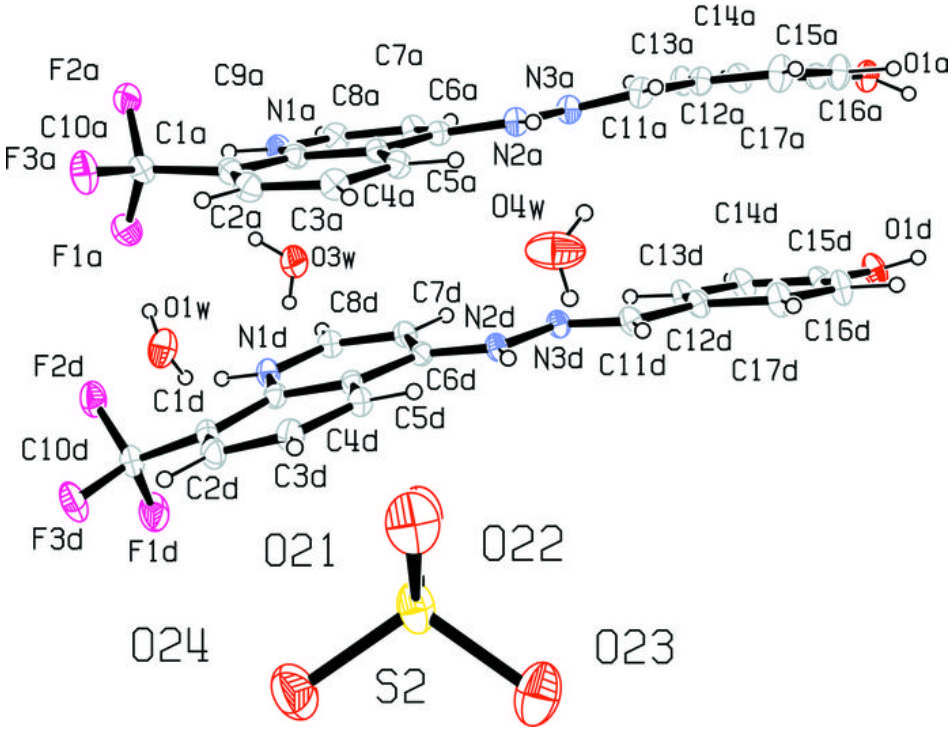
C9B—C1B—C10B—F2B	−61.3 (2)	C9D—C1D—C10D—F3D	176.19 (15)
C2B—C1B—C10B—F1B	−122.11 (18)	N2D—N3D—C11D—C12D	175.34 (13)
C9B—C1B—C10B—F1B	57.9 (2)	N3D—C11D—C12D—C17D	179.64 (16)
N2B—N3B—C11B—C12B	175.40 (14)	N3D—C11D—C12D—C13D	−3.1 (2)
N3B—C11B—C12B—C13B	15.0 (3)	C17D—C12D—C13D—C14D	0.9 (3)
N3B—C11B—C12B—C17B	−162.93 (18)	C11D—C12D—C13D—C14D	−176.46 (16)
C17B—C12B—C13B—C14B	−0.1 (3)	C12D—C13D—C14D—C15D	−0.7 (3)
C11B—C12B—C13B—C14B	−178.04 (16)	C13D—C14D—C15D—O1D	179.32 (16)
C12B—C13B—C14B—C15B	2.0 (3)	C13D—C14D—C15D—C16D	0.0 (3)
C13B—C14B—C15B—O1B	179.48 (19)	O1D—C15D—C16D—C17D	−178.83 (17)
C13B—C14B—C15B—C16B	−2.0 (3)	C14D—C15D—C16D—C17D	0.5 (3)
O1B—C15B—C16B—C17B	178.7 (2)	C15D—C16D—C17D—C12D	−0.3 (3)
C14B—C15B—C16B—C17B	0.1 (3)	C13D—C12D—C17D—C16D	−0.4 (3)
C15B—C16B—C17B—C12B	1.8 (4)	C11D—C12D—C17D—C16D	176.94 (17)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4W—H4W1···O11^{i}	0.835 (18)	2.23 (3)	2.986 (2)	151 (5)
N2A—H2AB···O11^{i}	0.88	1.99	2.8592 (18)	170
C4A—H4AA···O11^{i}	0.95	2.28	3.199 (2)	163
O1A—H1A···O12^{ii}	0.84	1.89	2.6677 (18)	154
O1D—H1D···O13^{ii}	0.84	1.75	2.5771 (17)	167
O4W—H4W2···O14^{iii}	0.820 (19)	2.06 (2)	2.860 (2)	167 (5)
C4D—H4DA···O14^{iii}	0.95	2.50	3.367 (2)	152
C11D—H11D···O14^{iii}	0.95	2.52	3.272 (2)	136
N1A—H1AA···O21^{i}	0.88	2.06	2.8636 (18)	151
O3W—H3W2···O22^{i}	0.841 (18)	2.039 (19)	2.864 (2)	167 (4)
N2B—H2BB···O22^{iv}	0.88	1.93	2.7909 (18)	166
C4B—H4BA···O22^{iv}	0.95	2.37	3.294 (2)	165
C11B—H11B···O22^{iv}	0.95	2.55	3.319 (2)	138
O3W—H3W1···O23^{iii}	0.824 (18)	1.952 (19)	2.776 (2)	179 (5)
O1W—H1W1···O24^{iii}	0.810 (17)	1.933 (17)	2.725 (2)	165 (3)
C8A—H8AA···O24^{i}	0.95	2.39	3.134 (2)	135
C7C—H7CA···O1A^{v}	0.95	2.46	3.0647 (19)	122
C8C—H8CA···O1A^{v}	0.95	2.47	3.078 (2)	122
O2W—H2W1···O1D^{vi}	0.821 (17)	2.114 (18)	2.933 (2)	175 (4)
C8B—H8BA···O1D^{v}	0.95	2.34	3.234 (2)	157
O1C—H1C···O3W^{v}	0.84	1.82	2.651 (2)	168
O2W—H2W2···O4W^{i}	0.828 (17)	1.931 (17)	2.759 (3)	177 (3)

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

Fig. 1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C1d
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O21
O22
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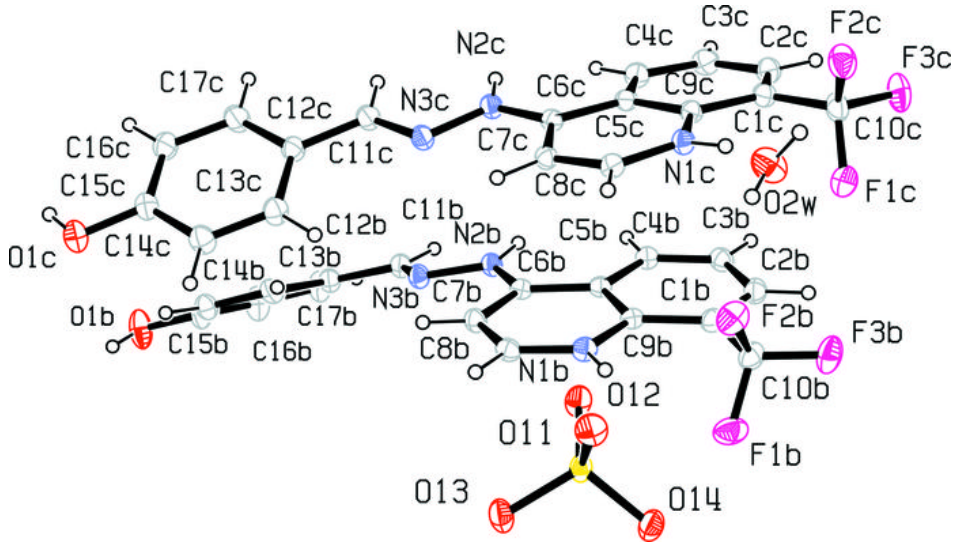
O23
S2

Fig. 2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C17b
F2b
F3b
C15b
C16b
C8b
C9b
N1b
C10b
O12
O11
F1b
O13
O14

Fig. 3