

A 1:1 co-crystal of quinol and pyridine

Iain D. H. Oswald,^{a*} W. D. Sam
Motherwell^b and Simon Parsons^a^aSchool of Chemistry, The University of
Edinburgh, King's Buildings, West Mains Road,
Edinburgh EH9 3JJ, Scotland, and ^bCambridge
Crystallographic Data Centre, 12 Union Road,
Cambridge CB2 1EZ, England

Correspondence e-mail: iain.oswald@ed.ac.uk

Key indicators

Single-crystal X-ray study

T = 150 K

Mean $\sigma(\text{C}-\text{C}) = 0.002 \text{ \AA}$

R factor = 0.048

wR factor = 0.120

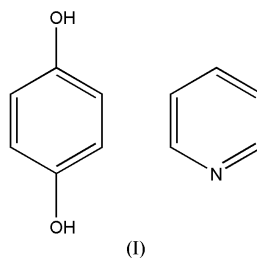
Data-to-parameter ratio = 16.7

For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

A co-crystal of quinol and pyridine would be expected to form with 1:2 stoichiometry because quinol has two hydrogen-bond donors and pyridine has one hydrogen-bond acceptor which is more basic than phenolic oxygen. We report the structure of a 1:1 co-crystal, *viz.* quinol–pyridine (1/1), $\text{C}_6\text{H}_6\text{O}_2 \cdot \text{C}_5\text{H}_5\text{N}$, which does not conform to this expectation. Its stability appears to imply that a combination of individually relatively weak $\text{C}-\text{H} \cdots \text{O}$, $\text{C}-\text{H} \cdots \pi$ and $\pi-\pi$ stacking interactions are energetically competitive with $\text{O}-\text{H} \cdots \text{N}$ hydrogen bonds. Quinol molecules lie on inversion centres, while pyridine is in a general position.

Comment

Quinol shows a great propensity for forming co-crystals, and it is widely used to stabilize compounds that are susceptible to polymerization. A search of the Cambridge Structural Database (CSD, Version 5.25; Allen & Motherwell, 2002) shows that there are 92 co-crystals of quinol with a range of organic compounds. Of all these structures in the CSD, over half contain hydrogen-bond acceptors, *e.g.* 1,4-dioxane (Barnes *et al.*, 1990). We have recently reported (Oswald *et al.*, 2004) a series of crystal structures of co-crystals of quinol with pyrazine, piperazine, morpholine, pyridine, piperidine and 4,4'-bi-pyridine (hereafter referred to as guest molecules). These all have closely related packing motifs in which pairs of quinol and guest molecules are connected *via* $\text{N}-\text{H} \cdots \text{O}$ or $\text{C}-\text{H} \cdots \text{O}$ interactions.



Amine N atoms are more strongly basic than phenol O atoms and the shortest, and by implication strongest, hydrogen bonds formed in our previous studies were those from a phenol OH donor to an amine or a pyridine N atom. Pyrazine and piperazine, which both have two acceptor sites per molecule, were found to form 1:1 co-crystals with quinol, which contains two strong donor functions. In the co-crystals of quinol with molecules with N, NH or NMe and O, CH or CH_2 , respectively in the 1 and 4 positions of a six-membered ring, quinol was found to form hydrogen bonds exclusively to the nitrogen moiety, promoting the formation of quinol–guest co-crystals in a 1:2 ratio. This trend is exemplified by pyridine,

Received 24 August 2004

Accepted 30 September 2004

Online 9 October 2004

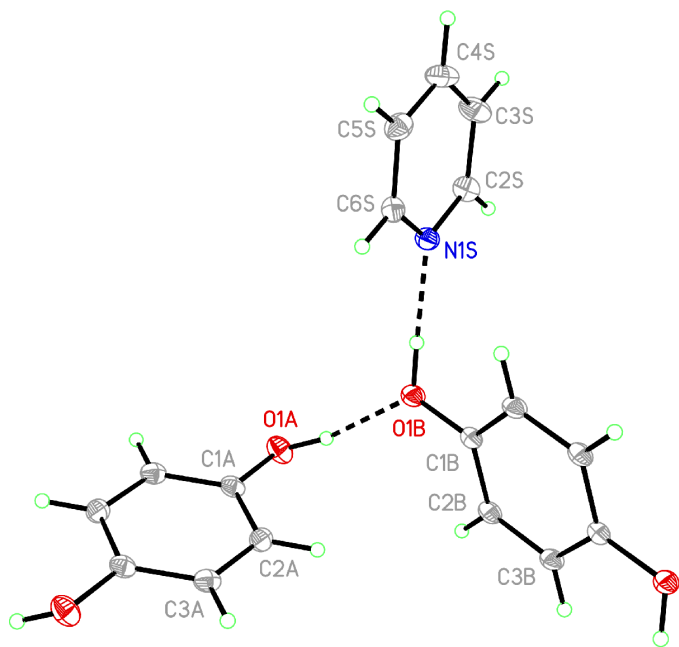


Figure 1
Displacement ellipsoid plot of (I), showing the two crystallographically independent quinol molecules (labelled *A* and *B*) and the pyridine molecule (labelled *S*). Ellipsoids are drawn at the 30% probability level.

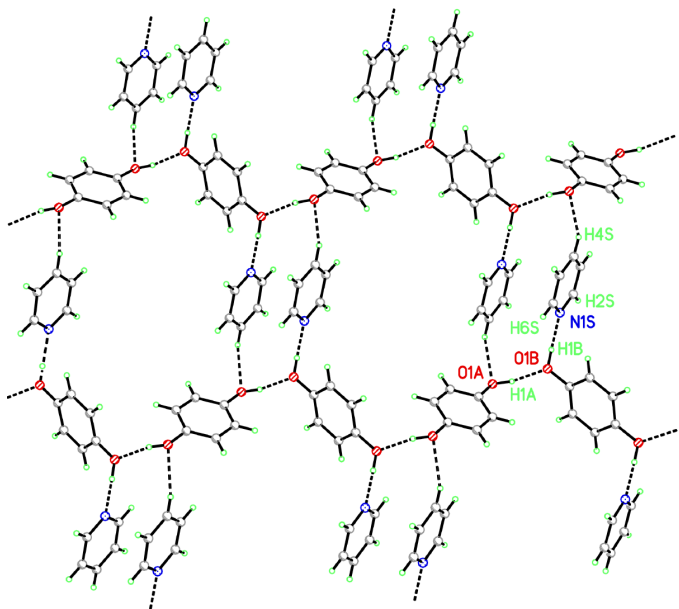


Figure 2
Strong O—H...O hydrogen bonds connect quinol molecules into chains. Pyridine molecules are connected on either side of the chains by O—H...N hydrogen bonds. π – π Stacking and C—H...O interactions involving the pyridine molecules also link the chains into a layer. The O—H...O and O—H...N hydrogen bonds are shown as heavy dashed lines and the weaker C—H...O interactions as open dashes. This view is along the $(\bar{1}12)$ reciprocal lattice direction.

which forms a co-crystal containing quinol and pyridine in 1:2 ratio.

In this paper, we report the crystal structure of a 1:1 co-crystal of quinol and pyridine, (I), which is an exception to the general stoichiometry rules described above. It was obtained

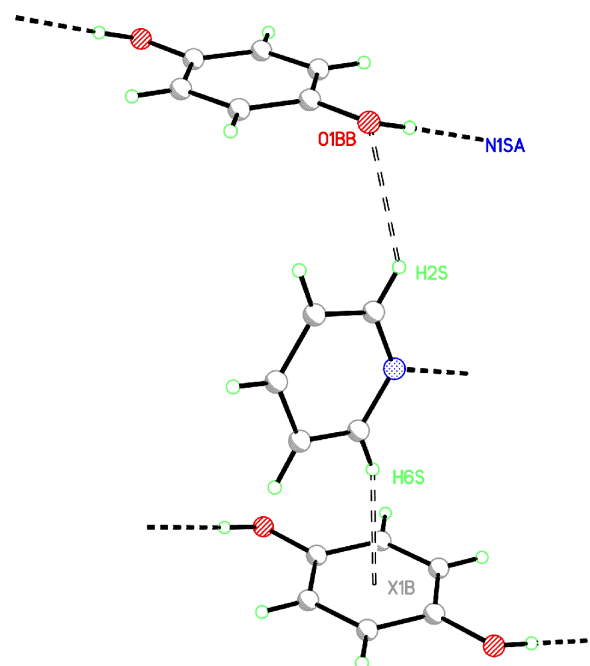


Figure 3
The layers (see Fig. 2) are connected through C—H... π and C—H...O interactions to the layers above and below. X1B is the centroid of the benzene ring (see Table 1). This view is along $[010]$.

by refluxing and then cooling a solution of quinol dissolved in a minimum quantity of pyridine.

Co-crystal (I) crystallizes in space group $P\bar{1}$ and the asymmetric unit consists of one molecule of pyridine in a general position and two half-molecules of quinol (labelled *A* and *B*) residing on crystallographic inversion centres (Fig. 1). Primary bond distances and angles are normal and are listed in the deposited CIF.

The shortest and strongest intermolecular interactions in the structure are O—H...O and O—H...N hydrogen bonds (Fig. 2 and Table 1). Quinol molecules *A* and *B* alternate along a chain built by O—H...O hydrogen bonds, in which molecule *A* provides the OH-donor functions, while molecule *B* acts as the acceptor. The chains run along the $[110]$ direction and form a $C_2^2(14)$ graph set (Bernstein *et al.*, 1995). Molecule *B* donates to pairs of pyridine molecules, which lie on either side of the chain. Successive pyridine molecules are related by the $\bar{1}$ operations centred in the middle of the quinol rings. Co-crystal (I) is the only co-crystal in our study that we have observed in which quinol molecules are directly hydrogen bonded to one another.

The only conventional hydrogen-bonding function 'unsatisfied' by the N—H...O and O—H...O hydrogen bonding described above is the phenol O atom of molecule *A*. There is a close contact between this phenol group and a pyridine attached to an adjacent chain (C4S—H4S...O1A = 2.57 Å and 127°).

Inter-chain connections are also formed by π – π stacking between pairs of pyridine molecules. The distance between the atoms in one ring and the mean plane of the other varies in the range 3.532–3.538 (2) Å; the planes are exactly parallel by

symmetry. The symmetry code relating the rings in this interaction is $(2 - x, 1 - y, -z)$.

The C4S—H4S···O1A and π – π stacking interactions connect the chains into a layer parallel to $(\bar{1}12)$. The layers are stacked, with quinol molecules above and below the rather ‘open’ region between the pairs of π -stacked pyridine rings in Fig. 2. The layers are connected in this region by C6S—H6S··· π and C2S—H2S···O1B interactions, where the π acceptor is the aromatic ring from a quinol (molecule B, see Fig. 3). The distance between H6S and the centroid of the benzene ring (*X1B*) in this interaction is 2.53 Å, with an angle of 162° subtended at the H atom. The weak C2S—H2S···O1B interaction measures 2.69 Å, with an angle at H2S of 136°.

C—H···O hydrogen bonding is now widely accepted (Desiraju & Steiner, 1999), and weak hydrogen bonding can be exploited in supramolecular chemistry and crystal structure design. For example, C—H···O bonds may play a very important role in protein folding (Derewenda *et al.*, 1995). The CH groups in pyridine rings are often observed to act as donor groups in CH···acceptor interactions. Related interactions also occur in heterocyclic compounds related to pyridine, for example, in quinol–pyrazine (Oswald *et al.*, 2004). Such interactions are strong enough that they can be used in crystal engineering, as demonstrated, for example, by Bond (2003) in a series of co-crystals of pyrazine with carboxylic acids. π – π Stacking has also been observed to be competitive with conventional hydrogen bonding in, for example, the 1:2 co-crystal of quinol with 4,4'-bipyridine (Oswald *et al.*, 2004).

That a co-crystal with 1:1 stoichiometry should be obtained from a mixture of quinol and pyridine must imply that the combination of C—H···O, π – π stacking and C—H··· π interactions is competitive with O—H···N hydrogen bonding, even for a relatively basic centre such as pyridine.

Experimental

Starting materials were obtained from Sigma–Aldrich and were used as received. Quinol (0.49 g, 4.45 mmol) was refluxed in a minimum volume of pyridine to dissolve the solid. The solution was allowed to cool to room temperature to produce colourless blocks.

Crystal data

$C_6H_6O_2 \cdot C_5H_5N$	$Z = 2$
$M_r = 189.21$	$D_x = 1.310 \text{ Mg m}^{-3}$
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 5.7451 (5) \text{ \AA}$	Cell parameters from 2033 reflections
$b = 9.1570 (9) \text{ \AA}$	$\theta = 2\text{--}29^\circ$
$c = 9.6247 (9) \text{ \AA}$	$\mu = 0.09 \text{ mm}^{-1}$
$\alpha = 89.002 (2)^\circ$	$T = 150 (2) \text{ K}$
$\beta = 76.222 (2)^\circ$	Block, colourless
$\gamma = 77.478 (2)^\circ$	$0.33 \times 0.18 \times 0.18 \text{ mm}$
$V = 479.76 (8) \text{ \AA}^3$	

Data collection

Bruker SMART APEX CCD area-detector diffractometer with Cryostream cooler (Cosier & Glazer, 1986)	4349 measured reflections 2248 independent reflections 1853 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.018$ $\theta_{\text{max}} = 28.7^\circ$
ω scans	$h = -7 \rightarrow 7$
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)	$k = -12 \rightarrow 12$
$T_{\text{min}} = 0.841, T_{\text{max}} = 0.980$	$l = -12 \rightarrow 13$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.049P)^2 + 0.1585P]$
$R[F^2 > 2\sigma(F^2)] = 0.048$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.120$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.04$	$\Delta\rho_{\text{max}} = 0.28 \text{ e \AA}^{-3}$
2248 reflections	$\Delta\rho_{\text{min}} = -0.21 \text{ e \AA}^{-3}$
135 parameters	
H atoms treated by a mixture of independent and constrained refinement	

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

$D\text{--}H\cdots A$	$D\text{--}H$	$H\cdots A$	$D\cdots A$	$D\text{--}H\cdots A$
O1A—H1A···O1B ⁱ	0.94 (3)	1.81 (3)	2.7392 (16)	168 (2)
O1B—H1B···N1S ⁱⁱ	0.93 (2)	1.79 (2)	2.7178 (17)	178 (2)
C2S—H2S···O1B	0.95	2.69	3.436 (2)	136
C4S—H4S···O1A	0.95	2.57	3.225 (2)	127
C6S—H6S···X1B ⁱⁱⁱ	0.95	2.53	3.45	162

Symmetry codes: (i) $1 + x, y, z$; (ii) $1 - x, 1 - y, -z$; (iii) $1 + x, y, z - 1$. *X1B* is the centroid of the benzene ring.

H atoms were placed on C atoms in calculated positions (C—O = 0.95 Å) and allowed to ride on their parent atoms [$U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$]. Hydroxyl H atoms were located in difference maps and refined freely.

Data collection: SMART (Bruker–Nonius, 2001); cell refinement: SAINT (Bruker–Nonius, 2003); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2001); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL, PLATON [Spek (2004) as incorporated in WinGX (Farrugia, 1999)] and enCIFer (Version 1.1; Allen *et al.*, 2004).

The authors thank the EPSRC, The University of Edinburgh and The Cambridge Crystallographic Data Centre for funding.

References

- Allen, F. H., Johnson, O., Shields, G. P., Smith, B. R. & Towler, M. (2004). *J. Appl. Cryst.* **37**, 335–338.
- Allen, F. H. & Motherwell, W. D. S. (2002). *Acta Cryst.* **B58**, 407–422.
- Barnes, J. C., Paton, J. D. & Blyth, C. S. (1990). *Acta Cryst.* **C46**, 1183–1184.
- Bernstein, J., Davis, R. E., Shimon, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
- Bond, A. D. (2003). *Chem. Commun.* pp. 250–251.
- Bruker–Nonius (2001). SMART. Version 5.624. Bruker–Nonius Inc., Madison, Wisconsin, USA.
- Bruker–Nonius (2003). SAINT. Version 7. Bruker–Nonius Inc., Madison, Wisconsin, USA.
- Cosier, J. & Glazer, A. M. (1986). *J. Appl. Cryst.* **19**, 105–107.
- Derewenda, Z. S., Lee, L. & Derewenda, U. (1995). *J. Mol. Biol.* **252**, 248–262.
- Desiraju, G. R. & Steiner, T. (1999). *The Weak Hydrogen Bond*. IUCr Monographs on Crystallography, No. 9. Oxford University Press.
- Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
- Oswald, I. D. H., Motherwell, W. D. S. & Parsons, S. (2004). *Acta Cryst.* **B60**. Submitted.
- Sheldrick, G. M. (2001). SHELXTL. Version 6.01. Bruker–Nonius Inc., Madison, Wisconsin, USA.
- Sheldrick, G. M. (2004). SADABS. University of Göttingen, Germany.
- Spek, A. L. (2004). PLATON. Utrecht University, The Netherlands.

supporting information

Acta Cryst. (2004). E60, o1967–o1969 [https://doi.org/10.1107/S1600536804024547]

A 1:1 co-crystal of quinol and pyridine

Iain D. H. Oswald, W. D. Sam Motherwell and Simon Parsons

Quinol–Pyridine (1/1)

Crystal data

$C_6H_6O_2 \cdot C_5H_5N$	$Z = 2$
$M_r = 189.21$	$F(000) = 200$
Triclinic, $P\bar{1}$	$D_x = 1.310 \text{ Mg m}^{-3}$
Hall symbol: $-P1$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 5.7451 (5) \text{ \AA}$	Cell parameters from 2033 reflections
$b = 9.1570 (9) \text{ \AA}$	$\theta = 2\text{--}29^\circ$
$c = 9.6247 (9) \text{ \AA}$	$\mu = 0.09 \text{ mm}^{-1}$
$\alpha = 89.002 (2)^\circ$	$T = 150 \text{ K}$
$\beta = 76.222 (2)^\circ$	Block, colourless
$\gamma = 77.478 (2)^\circ$	$0.33 \times 0.18 \times 0.18 \text{ mm}$
$V = 479.76 (8) \text{ \AA}^3$	

Data collection

Bruker APEX CCD area-detector diffractometer	4349 measured reflections
Radiation source: fine-focus sealed tube	2248 independent reflections
Graphite monochromator	1853 reflections with $I > 2\Sigma(I)$
ω scans	$R_{\text{int}} = 0.018$
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)	$\theta_{\text{max}} = 28.7^\circ$, $\theta_{\text{min}} = 2.2^\circ$
$T_{\text{min}} = 0.841$, $T_{\text{max}} = 0.980$	$h = -7 \rightarrow 7$
	$k = -12 \rightarrow 12$
	$l = -12 \rightarrow 13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: geom and difmap (OH)
$R[F^2 > 2\sigma(F^2)] = 0.048$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.120$	$w = 1/[\sigma^2(F_o^2) + (0.049P)^2 + 0.1585P]$
$S = 1.04$	where $P = (F_o^2 + 2F_c^2)/3$
2248 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
135 parameters	$\Delta\rho_{\text{max}} = 0.28 \text{ e \AA}^{-3}$
0 restraints	$\Delta\rho_{\text{min}} = -0.21 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All s.u.s 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. S.u.s are not quoted for interactions involving calculated H-atom positions.

Refinement. 912_ALERT_3_B Missing FCF Reflections Above STH/L=0.6 228 911_ALERT_3_C Missing FCF Refl. Between TH(Min) & STH/L=0.6.. 8
Not serious. Coverage statistics:

Resolution & Completeness Statistics (Cumulative)

sin(theta)/Lambda Complete Expected Measured Missing ----- Theta

20.82 0.500 1.000 1004 1004 0 23.01 0.550 0.998 1334 1331 3 25.24 0.600 0.995 1734 1726 8 -----
----- ACTA Min. Res. --- 27.51 0.650 0.975 2208 2152 56 29.84 0.700 0.905 2484 2248 236

061_ALERT_3_C Tmax/Tmin Range Test RR' too Large 0.87

Tmin and Tmax reported: 0.841 0.980 Tmin' and Tmax expected: 0.970 0.984

Noted, but no action taken. SADABS attempts to correct for all systematic errors not just absorption. The large range could represent a small amount of crystal decay for example.

480_ALERT_4_C Long H...A H-Bond Reported H2S.. O1B.. 2.69 A ng.

See text.

716_ALERT_1_C H...A Unknown or Inconsistent Label X1B H6S X1B 718_ALERT_1_C D—H..A Unknown or Inconsistent Label X1B C6S H6S X1B

See Table 1 and Figure 3.

764_ALERT_4_C Overcomplete CIF Bond List Detected (Rep/Expd). 1.14 Ratio

Noted; no action taken. The quinol molecules are on -1 sites, which may explain why this has happened.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	U_{iso}^*/U_{eq}
O1A	1.3232 (2)	0.07757 (13)	0.26274 (12)	0.0362 (3)
H1A	1.344 (4)	0.174 (3)	0.281 (2)	0.065 (7)*
C1A	1.1638 (3)	0.04088 (16)	0.38221 (16)	0.0263 (3)
C2A	1.1609 (3)	0.08591 (16)	0.51998 (17)	0.0278 (3)
H2A	1.2717	0.1445	0.5340	0.033*
C3A	0.9969 (3)	0.04557 (16)	0.63687 (16)	0.0283 (3)
H3A	0.9948	0.0775	0.7306	0.034*
O1B	0.3575 (2)	0.36954 (12)	0.28535 (12)	0.0290 (3)
H1B	0.268 (4)	0.441 (3)	0.238 (2)	0.057 (6)*
C1B	0.4247 (3)	0.43589 (16)	0.39227 (15)	0.0239 (3)
C2B	0.6167 (3)	0.35608 (16)	0.44644 (16)	0.0256 (3)
H2B	0.6960	0.2573	0.4106	0.031*
C3B	0.6928 (3)	0.42029 (16)	0.55269 (16)	0.0252 (3)
H3B	0.8258	0.3657	0.5881	0.030*
N1S	0.8953 (2)	0.41739 (14)	-0.14401 (14)	0.0283 (3)
C2S	0.8062 (3)	0.34857 (18)	-0.02635 (17)	0.0330 (4)
H2S	0.6370	0.3800	0.0198	0.040*
C3S	0.9484 (4)	0.2340 (2)	0.03146 (18)	0.0408 (4)
H3S	0.8787	0.1883	0.1160	0.049*
C4S	1.1934 (4)	0.1870 (2)	-0.03559 (19)	0.0398 (4)
H4S	1.2952	0.1076	0.0013	0.048*
C5S	1.2883 (3)	0.25698 (19)	-0.15699 (18)	0.0348 (4)
H5S	1.4567	0.2272	-0.2052	0.042*
C6S	1.1336 (3)	0.37130 (18)	-0.20724 (17)	0.0300 (3)
H6S	1.1997	0.4196	-0.2909	0.036*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1A	0.0467 (7)	0.0270 (6)	0.0325 (6)	-0.0101 (5)	-0.0030 (5)	0.0004 (5)
C1A	0.0313 (8)	0.0171 (6)	0.0285 (8)	-0.0004 (6)	-0.0075 (6)	0.0016 (5)
C2A	0.0311 (8)	0.0199 (7)	0.0341 (8)	-0.0040 (6)	-0.0123 (6)	-0.0008 (6)
C3A	0.0379 (8)	0.0202 (7)	0.0267 (7)	-0.0015 (6)	-0.0118 (6)	-0.0013 (5)
O1B	0.0364 (6)	0.0207 (5)	0.0317 (6)	-0.0040 (4)	-0.0136 (5)	0.0021 (4)
C1B	0.0261 (7)	0.0197 (7)	0.0258 (7)	-0.0054 (5)	-0.0057 (6)	0.0038 (5)
C2B	0.0269 (7)	0.0167 (7)	0.0303 (8)	-0.0008 (5)	-0.0051 (6)	0.0021 (5)
C3B	0.0244 (7)	0.0200 (7)	0.0296 (8)	-0.0011 (5)	-0.0070 (6)	0.0045 (5)
N1S	0.0329 (7)	0.0242 (6)	0.0292 (7)	-0.0052 (5)	-0.0110 (5)	0.0024 (5)
C2S	0.0351 (8)	0.0323 (8)	0.0288 (8)	-0.0043 (7)	-0.0048 (7)	0.0001 (6)
C3S	0.0556 (11)	0.0361 (9)	0.0266 (8)	-0.0049 (8)	-0.0072 (8)	0.0075 (7)
C4S	0.0510 (11)	0.0316 (9)	0.0353 (9)	0.0048 (8)	-0.0199 (8)	0.0011 (7)
C5S	0.0313 (8)	0.0348 (9)	0.0377 (9)	-0.0026 (7)	-0.0111 (7)	-0.0049 (7)
C6S	0.0329 (8)	0.0286 (8)	0.0317 (8)	-0.0111 (6)	-0.0098 (6)	0.0030 (6)

Geometric parameters (\AA , $^\circ$)

O1A—C1A	1.3755 (19)	C3B—C1B ⁱⁱ	1.392 (2)
O1A—H1A	0.94 (3)	C3B—H3B	0.9500
C1A—C3A ⁱ	1.384 (2)	N1S—C2S	1.334 (2)
C1A—C2A	1.391 (2)	N1S—C6S	1.336 (2)
C2A—C3A	1.386 (2)	C2S—C3S	1.379 (2)
C2A—H2A	0.9500	C2S—H2S	0.9500
C3A—C1A ⁱ	1.384 (2)	C3S—C4S	1.377 (3)
C3A—H3A	0.9500	C3S—H3S	0.9500
O1B—C1B	1.3745 (18)	C4S—C5S	1.377 (3)
O1B—H1B	0.93 (2)	C4S—H4S	0.9500
C1B—C2B	1.391 (2)	C5S—C6S	1.380 (2)
C1B—C3B ⁱⁱ	1.392 (2)	C5S—H5S	0.9500
C2B—C3B	1.389 (2)	C6S—H6S	0.9500
C2B—H2B	0.9500		
C1A—O1A—H1A	107.2 (14)	C2B—C3B—H3B	119.8
O1A—C1A—C3A ⁱ	118.11 (14)	C1B ⁱⁱ —C3B—H3B	119.8
O1A—C1A—C2A	122.49 (14)	C2S—N1S—C6S	117.48 (14)
C3A ⁱ —C1A—C2A	119.40 (14)	N1S—C2S—C3S	123.05 (16)
C3A—C2A—C1A	120.20 (14)	N1S—C2S—H2S	118.5
C3A—C2A—H2A	119.9	C3S—C2S—H2S	118.5
C1A—C2A—H2A	119.9	C4S—C3S—C2S	118.77 (16)
C1A ⁱ —C3A—C2A	120.40 (14)	C4S—C3S—H3S	120.6
C1A ⁱ —C3A—H3A	119.8	C2S—C3S—H3S	120.6
C2A—C3A—H3A	119.8	C5S—C4S—C3S	118.90 (16)
C1B—O1B—H1B	110.5 (14)	C5S—C4S—H4S	120.6
O1B—C1B—C2B	118.52 (13)	C3S—C4S—H4S	120.6
O1B—C1B—C3B ⁱⁱ	122.17 (13)	C4S—C5S—C6S	118.62 (16)

C2B—C1B—C3B ⁱⁱ	119.31 (14)	C4S—C5S—H5S	120.7
C3B—C2B—C1B	120.23 (13)	C6S—C5S—H5S	120.7
C3B—C2B—H2B	119.9	N1S—C6S—C5S	123.18 (15)
C1B—C2B—H2B	119.9	N1S—C6S—H6S	118.4
C2B—C3B—C1B ⁱⁱ	120.45 (13)	C5S—C6S—H6S	118.4

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

Hydrogen-bond geometry (Å, °)

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
O1A—H1A...O1B ⁱⁱⁱ	0.94 (3)	1.81 (3)	2.7392 (16)	168 (2)
O1B—H1B...N1S ^{iv}	0.93 (2)	1.79 (2)	2.7178 (17)	178 (2)
C2S—H2S...O1B	0.95	2.69	3.436 (2)	136
C4S—H4S...O1A	0.95	2.57	3.225 (2)	127
C6S—H6S...X1B ^v	0.95	2.53	3.45	162

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