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ISSN 2414-3146

# Bis(2-aminobenzimidazolium) sulfate monohydrate

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Received 15 December 2021
Accepted 14 February 2022

Edited by W. T. A. Harrison, University of Aberdeen, Scotland

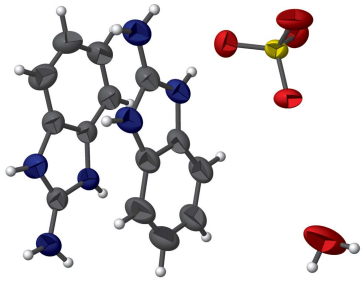
**Keywords:** crystal structure; 2-aminobenzimidazolium; sulfate.

**CCDC reference**: 1810894

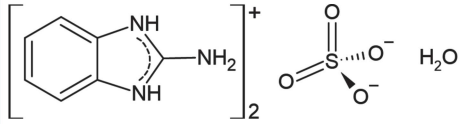
**Structural data**: full structural data are available from iucrdata.iucr.org

In the title hydrated molecular salt, $2C_7H_8N_3^+\cdot SO_4^{2-}\cdot H_2O$, the components are linked by numerous N—H···O and O—H···O hydrogen bonds.

**3D view**



**Chemical scheme**




## Structure description

2-Aminobenzimidazole has been used for the synthesis of a series of sulfur heterocycles such as 9*H*-3-thia-1,4a,9-triaza-fluorene-2,4-dithione (**1**): its potassium thiolate salt was used to prepare metal coordination compounds (Peña-Hueso *et al.*, 2008), and is the precursor of the title compound. When compound **1** is dissolved in dimethyl sulfoxide and strong acids are added, instead of producing the protonated derivative, the thiadiazine ring breaks down, producing 2-aminobenzimidazolium sulfate (**2**): its crystal structural features are the subject of the present paper.

Compound **2** is formed by the transfer of two protons from sulfuric acid to the heterocycle: the crystal has two 2-aminobenzimidazolium cations, one sulfate anion and one water molecule in its asymmetric unit (Fig. 1). There is a small asymmetry in the S—O bond lengths of the $SO_4^{2-}$ ion from 1.4596 (16) to 1.4723 (15) Å, probably caused by the hydrogen bonds around the anion (Gagné & Hawthorne, 2018). Two benzimidazolium cations are stacked in a head-to-tail way, with a distance between C9 of one molecule and C18 of another of 3.441 (3) Å.

The sulfate ion accepts seven N—H···O hydrogen bonds from four adjacent benzimidazolium cations and one O—H···O link from a water molecule (Table 1, Fig. 2). The water molecule accepts one N—H···O hydrogen bond and forms two O—H···O links to two $SO_4^{2-}$ ions (Fig. 3). In the extended structure, the benzimidazolium cations form parallel ribbons propagating in the [010] direction (Fig. 4).

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···O25$^{i}$ | 0.81 (4) | 2.25 (3) | 2.946 (3) | 144 (3) |
| N3—H3···O22$^{ii}$ | 0.83 (3) | 1.93 (3) | 2.749 (3) | 172 (3) |
| N11—H11···O23 | 0.85 (4) | 1.96 (4) | 2.786 (4) | 166 (3) |
| N13—H13···O24$^{iii}$ | 0.83 (4) | 1.91 (4) | 2.720 (3) | 165 (3) |
| N10—H101···O23$^{i}$ | 0.87 (4) | 2.03 (4) | 2.894 (5) | 169 (3) |
| N10—H102···O25$^{ii}$ | 0.89 (3) | 2.00 (3) | 2.890 (3) | 175 (3) |
| N20—H201···O26$^{iii}$ | 0.84 (3) | 2.04 (3) | 2.853 (4) | 165 (3) |
| N20—H202···O22$^{iii}$ | 0.93 (4) | 2.09 (4) | 2.973 (4) | 157 (3) |
| O26—H261···O24$^{iv}$ | 0.80 (7) | 2.22 (7) | 2.983 (4) | 160 (7) |
| O26—H262···O24$^{v}$ | 0.80 (7) | 2.14 (7) | 2.860 (4) | 150 (6) |
| C17—H17···O22 | 0.95 | 2.56 | 3.272 (3) | 132 |

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

The first crystal structure of a 2-aminobenzimidazolium salt was reported with the nitrate anion (Bats *et al.*, 1999) and a related structure with hydrogen sulfate as the counter-ion is also known (You *et al.*, 2009).

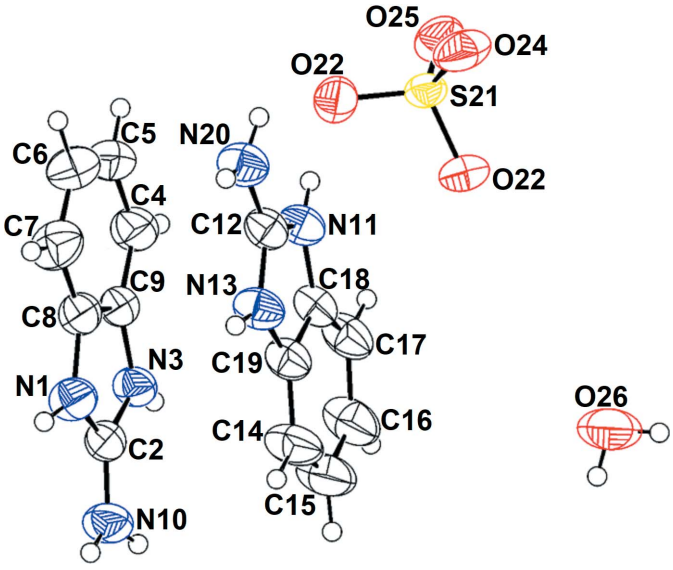



**Figure 1**
The molecular structure of **2** showing displacement ellipsoids drawn at the 50% probability level

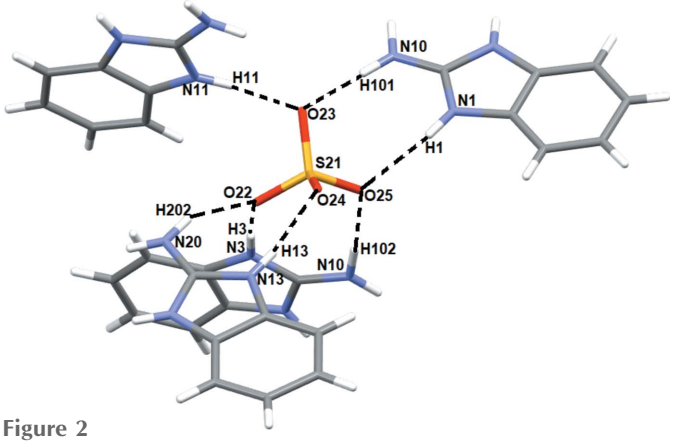



**Figure 2**
Hydrogen-bond environment around the sulfate anion.

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $2C_7H_8N_3^+\cdot SO_4^{2-}\cdot H_2O$ |
| $M_r$ | 382.4 |
| Crystal system, space group | Monoclinic, $P2_1/c$ |
| Temperature (K) | 293 |
| $a, b, c$ (Å) | 12.1115 (2), 10.6282 (2), 17.4772 (3) |
| $\beta$ (°) | 127.723 (1) |
| $V$ (Å$^3$) | 1779.48 (6) |
| $Z$ | 4 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.22 |
| Crystal size (mm) | 0.25 × 0.25 × 0.17 |
| | |
| Data collection | |
| Diffractometer | Nonius KappaCCD |
| No. of measured, independent and observed [$I > 3.0\sigma(I)$] reflections | 9132, 4563, 2429 |
| $R_{int}$ | 0.04 |
| $(\sin\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.675 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.041, 0.050, 1.03 |
| No. of reflections | 2429 |
| No. of parameters | 265 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.25, −0.31 |

Computer programs: *COLLECT* (Nonius, 2001), *DENZO*/*SCALEPACK* (Otwinowski & Minor, 1997), *SHELXS97* (Sheldrick, 2008), *CRYSTALS* (Betteridge *et al.*, 2003) and *CAMERON* (Watkin *et al.*, 1996).

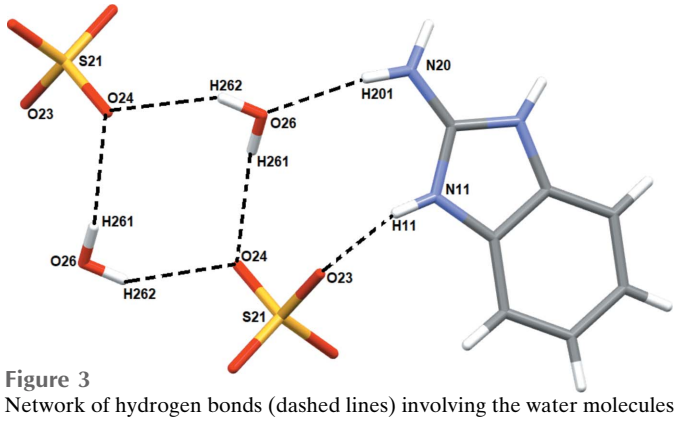



**Figure 3**
Network of hydrogen bonds (dashed lines) involving the water molecules and sulfate ions.

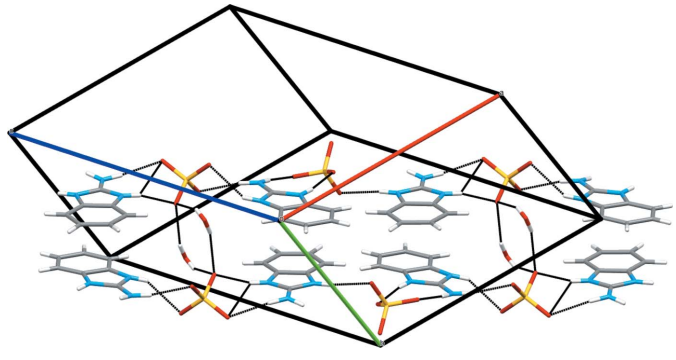


**Figure 4**
The unit-cell packing showing [010] ribbons of cations linked by sulfate anions.

## Synthesis and crystallization

The decomposition of 9*H*-3-thia-1,4a,9-triaza-fluorene-2,4-dithione with dilute aqueous $H_2SO_4$ in DMSO afforded the title compound **2**, m.p. 287–289°C. IR (KBr), $\nu$ ($cm^{-1}$): 3285 (N—H), 1682 (C═N), 1520 (C═C), 1478 (C—N). NMR (DMSO-$d_6$, p.p.m.) $\delta$ $^1$H: 7.27 (H4, H7); 7.09 (H5, H6); 13.18 (N1—H, N3—H); 8.70 ($NH_2$). $\delta$ $^{13}$C: 152.1 (C2); 111.8 (C4, C7); 123.4 (C5, C6); 130.4 (C8, C9). $\delta$ $^{15}$N: −257.1 (N1, N3); −312.9 (N10). Analysis calculated (%) for $C_{16}H_{16}N_6SO_5$: C, 43.97; H, 4.74; N, 21.98. Found: C, 43.50; H, 4.80; N, 21.80. The chemical shifts of C2 (152.1 p.p.m.), C8 and C9 (130.4 p.p.m.) in the $^{13}$C NMR spectrum indicate that the endocyclic nitrogen atoms are protonated, in agreement with the crystal structure.

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.


## Funding information

The authors thank Cinvestav for financial support.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# full crystallographic data

*IUCrData* (2022). **7**, x220172 [https://doi.org/10.1107/S2414314622001729]

## Bis(2-aminobenzimidazolium) sulfate monohydrate

**Adrian Peña Hueso, Adriana Esparza Ruiz and Angelina Flores Parra**

### Bis(2-aminobenzimidazolium) sulfate monohydrate

*Crystal data*

$2C_7H_8N_3^+\cdot SO_4^{2-}\cdot H_2O$
$M_r$ = 382.4
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a$ = 12.1115 (2) Å
$b$ = 10.6282 (2) Å
$c$ = 17.4772 (3) Å
$\beta$ = 127.723 (1)°
$V$ = 1779.48 (6) Å$^3$
$Z$ = 4
$F(000)$ = 800
$D_x$ = 1.427 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 4784 reflections
$\theta$ = 1–29°
$\mu$ = 0.22 mm$^{-1}$
$T$ = 293 K
Prism, colourless
0.25 × 0.25 × 0.17 mm

*Data collection*

Nonius KappaCCD diffractometer
Radiation source: Enraf Nonius FR590
Graphite monochromator
Detector resolution: 9 pixels mm$^{-1}$
$\varphi$ & $\omega$ scans
9132 measured reflections
4563 independent reflections
2429 reflections with $I > 3.0\sigma(I)$
$R_{int}$ = 0.04
$\theta_{max}$ = 28.7°, $\theta_{min}$ = 2.1°
$h$ = −15→16
$k$ = −14→14
$l$ = −23→23

*Refinement*

Refinement on $F$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.050
$S$ = 1.03
2429 reflections
265 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
H atoms treated by a mixture of independent and constrained refinement
Method, part 1, Chebychev polynomial, (Watkin, 1994, *P*rince, 1982) [*w*eight] = $1.0/[A_0*T_0(x) + A_1*T_1(x) \cdots + A_{n-1}]*T_{n-1}(x)]$ where $A_i$ are the Chebychev coefficients listed below and x = $F$ /$F$max Method = Robust Weighting (*P*rince, 1982) W = [*w*eight] * [1-(delta$F$/6*sigma$F$)$^2$]$^2$ $A_i$ are: 0.914 0.838 0.564 0.170 0.849E-01
$(\Delta/\sigma)_{max}$ = 0.0002
$\Delta\rho_{max}$ = 0.25 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.31 e Å$^{-3}$

*Special details*

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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.
The positions of all NH and OH hydrogen atoms were refined, and all CH were placed at ideal positions.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C2 | 0.5660 (3) | 0.1533 (2) | −0.12552 (17) | 0.0484 |
| C4 | 0.5449 (3) | 0.1836 (2) | 0.0688 (2) | 0.0626 |
| C5 | 0.6271 (4) | 0.1200 (3) | 0.1556 (2) | 0.0725 |
| C6 | 0.7293 (3) | 0.0372 (3) | 0.1756 (2) | 0.0728 |
| C7 | 0.7524 (3) | 0.0132 (3) | 0.1090 (2) | 0.0682 |
| C8 | 0.6705 (3) | 0.0761 (2) | 0.02241 (18) | 0.0503 |
| C9 | 0.5691 (2) | 0.1616 (2) | 0.00250 (16) | 0.047 |
| C12 | 0.9604 (2) | 0.2887 (2) | 0.21087 (16) | 0.047 |
| C14 | 0.8306 (3) | 0.3839 (3) | −0.0275 (2) | 0.0719 |
| C15 | 0.7199 (4) | 0.4642 (3) | −0.0859 (2) | 0.0819 |
| C16 | 0.6467 (4) | 0.5164 (3) | −0.0557 (2) | 0.0786 |
| C17 | 0.6837 (3) | 0.4930 (3) | 0.03457 (18) | 0.0617 |
| C18 | 0.7951 (2) | 0.4131 (2) | 0.09334 (16) | 0.0479 |
| C19 | 0.8659 (3) | 0.3583 (2) | 0.06268 (17) | 0.0521 |
| H1 | 0.700 (3) | 0.023 (3) | −0.073 (2) | 0.0781* |
| H3 | 0.440 (3) | 0.256 (3) | −0.122 (2) | 0.0603* |
| H4 | 0.476 | 0.2396 | 0.0553 | 0.0818* |
| H5 | 0.6134 | 0.1333 | 0.2013 | 0.0945* |
| H6 | 0.7819 | −0.0041 | 0.2343 | 0.0851* |
| H7 | 0.82 | −0.0425 | 0.1215 | 0.0843* |
| H11 | 0.830 (3) | 0.384 (3) | 0.220 (2) | 0.0595* |
| H13 | 1.021 (3) | 0.235 (3) | 0.136 (2) | 0.0682* |
| H14 | 0.8797 | 0.3482 | −0.0463 | 0.0925* |
| H15 | 0.6943 | 0.4849 | −0.1462 | 0.0986* |
| H16 | 0.5679 | 0.568 | −0.0992 | 0.0857* |
| H17 | 0.6367 | 0.5309 | 0.0569 | 0.0697* |
| H101 | 0.580 (3) | 0.137 (3) | −0.227 (2) | 0.0811* |
| H102 | 0.472 (3) | 0.237 (3) | −0.247 (2) | 0.0806* |
| H201 | 1.041 (3) | 0.247 (3) | 0.339 (2) | 0.07* |
| H202 | 1.115 (3) | 0.183 (3) | 0.301 (2) | 0.0698* |
| H261 | 0.979 (7) | 0.918 (6) | 0.069 (5) | 0.1811* |
| H262 | 0.925 (6) | 0.838 (6) | 0.005 (5) | 0.1804* |
| N1 | 0.6657 (2) | 0.0745 (2) | −0.05947 (16) | 0.0562 |
| N3 | 0.5078 (2) | 0.20819 (19) | −0.08953 (14) | 0.0477 |
| N10 | 0.5301 (3) | 0.1737 (2) | −0.21296 (17) | 0.0601 |
| N11 | 0.85749 (19) | 0.3685 (2) | 0.18649 (14) | 0.0479 |
| N13 | 0.9688 (2) | 0.2826 (2) | 0.13810 (14) | 0.0539 |
| N20 | 1.0417 (2) | 0.2263 (2) | 0.29315 (16) | 0.0582 |

| | | | | |
|---|---|---|---|---|
| O22 | 0.72767 (16) | 0.64914 (16) | 0.21275 (11) | 0.0506 |
| O23 | 0.72874 (19) | 0.44104 (15) | 0.26788 (13) | 0.0584 |
| O24 | 0.8960 (2) | 0.5933 (2) | 0.37860 (12) | 0.0746 |
| O25 | 0.6554 (2) | 0.61476 (17) | 0.31313 (14) | 0.0657 |
| O26 | 0.9603 (4) | 0.8443 (3) | 0.06107 (18) | 0.1136 |
| S21 | 0.75054 (6) | 0.57563 (5) | 0.29273 (4) | 0.0431 |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C2 | 0.0604 (14) | 0.0435 (12) | 0.0537 (13) | 0.0027 (10) | 0.0411 (12) | −0.0021 (10) |
| C4 | 0.0850 (19) | 0.0550 (15) | 0.0668 (16) | 0.0109 (13) | 0.0563 (16) | 0.0013 (12) |
| C5 | 0.109 (2) | 0.0657 (17) | 0.0641 (17) | 0.0001 (17) | 0.0640 (18) | 0.0001 (14) |
| C6 | 0.087 (2) | 0.0733 (18) | 0.0555 (15) | 0.0049 (16) | 0.0420 (16) | 0.0142 (14) |
| C7 | 0.0703 (17) | 0.0651 (17) | 0.0705 (17) | 0.0194 (14) | 0.0436 (15) | 0.0185 (14) |
| C8 | 0.0577 (14) | 0.0464 (12) | 0.0551 (14) | 0.0060 (11) | 0.0388 (12) | 0.0017 (11) |
| C9 | 0.0580 (13) | 0.0411 (11) | 0.0484 (12) | 0.0015 (10) | 0.0358 (11) | −0.0010 (10) |
| C12 | 0.0421 (11) | 0.0541 (13) | 0.0449 (12) | −0.0005 (10) | 0.0266 (11) | −0.0062 (11) |
| C14 | 0.086 (2) | 0.087 (2) | 0.0555 (16) | 0.0163 (16) | 0.0498 (16) | −0.0027 (14) |
| C15 | 0.107 (3) | 0.085 (2) | 0.0498 (15) | 0.0272 (19) | 0.0461 (17) | 0.0063 (14) |
| C16 | 0.090 (2) | 0.0757 (19) | 0.0485 (15) | 0.0291 (17) | 0.0315 (15) | −0.0001 (14) |
| C17 | 0.0615 (15) | 0.0649 (16) | 0.0475 (14) | 0.0171 (13) | 0.0277 (12) | −0.0065 (12) |
| C18 | 0.0467 (12) | 0.0520 (13) | 0.0425 (12) | 0.0014 (10) | 0.0261 (11) | −0.0085 (10) |
| C19 | 0.0542 (14) | 0.0561 (14) | 0.0480 (13) | 0.0051 (11) | 0.0322 (12) | −0.0054 (11) |
| N1 | 0.0716 (14) | 0.0522 (12) | 0.0658 (13) | 0.0182 (11) | 0.0527 (12) | 0.0089 (10) |
| N3 | 0.0555 (11) | 0.0470 (10) | 0.0480 (11) | 0.0102 (9) | 0.0356 (10) | 0.0018 (9) |
| N10 | 0.0807 (16) | 0.0608 (13) | 0.0583 (13) | 0.0140 (11) | 0.0525 (13) | 0.0042 (10) |
| N11 | 0.0440 (10) | 0.0592 (12) | 0.0450 (10) | 0.0050 (9) | 0.0296 (9) | −0.0045 (9) |
| N13 | 0.0522 (12) | 0.0660 (13) | 0.0499 (11) | 0.0139 (10) | 0.0345 (10) | −0.0004 (10) |
| N20 | 0.0551 (12) | 0.0685 (14) | 0.0502 (12) | 0.0098 (11) | 0.0318 (11) | 0.0020 (11) |
| O22 | 0.0481 (9) | 0.0669 (10) | 0.0421 (8) | 0.0040 (7) | 0.0302 (8) | 0.0120 (7) |
| O23 | 0.0752 (12) | 0.0507 (9) | 0.0791 (12) | −0.0031 (8) | 0.0624 (11) | −0.0046 (8) |
| O24 | 0.0619 (11) | 0.1028 (15) | 0.0410 (9) | −0.0251 (11) | 0.0223 (9) | 0.0111 (9) |
| O25 | 0.0948 (14) | 0.0562 (10) | 0.0907 (13) | 0.0093 (9) | 0.0796 (12) | 0.0092 (9) |
| O26 | 0.144 (2) | 0.148 (3) | 0.0652 (14) | −0.069 (2) | 0.0725 (17) | −0.0286 (16) |
| S21 | 0.0483 (3) | 0.0508 (3) | 0.0396 (3) | −0.0046 (3) | 0.0317 (3) | 0.0008 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C2—N1 | 1.336 (3) | C15—H15 | 0.925 |
| C2—N3 | 1.333 (3) | C16—C17 | 1.374 (4) |
| C2—N10 | 1.326 (3) | C16—H16 | 0.95 |
| C4—C5 | 1.380 (4) | C17—C18 | 1.379 (3) |
| C4—C9 | 1.377 (3) | C17—H17 | 0.955 |
| C4—H4 | 0.931 | C18—C19 | 1.387 (3) |
| C5—C6 | 1.379 (4) | C18—N11 | 1.393 (3) |
| C5—H5 | 0.92 | C19—N13 | 1.389 (3) |
| C6—C7 | 1.378 (4) | H1—N1 | 0.80 (3) |

| | | | |
|---|---|---|---|
| C6—H6 | 0.922 | H3—N3 | 0.83 (3) |
| C7—C8 | 1.373 (4) | H11—N11 | 0.85 (3) |
| C7—H7 | 0.921 | H13—N13 | 0.83 (3) |
| C8—C9 | 1.390 (3) | H101—N10 | 0.87 (3) |
| C8—N1 | 1.396 (3) | H102—N10 | 0.89 (3) |
| C9—N3 | 1.386 (3) | H201—N20 | 0.83 (3) |
| C12—N11 | 1.343 (3) | H202—N20 | 0.93 (3) |
| C12—N13 | 1.338 (3) | H261—O26 | 0.81 (6) |
| C12—N20 | 1.321 (3) | H262—O26 | 0.79 (6) |
| C14—C15 | 1.376 (4) | O22—S21 | 1.4723 (15) |
| C14—C19 | 1.385 (4) | O23—S21 | 1.4711 (18) |
| C14—H14 | 0.919 | O24—S21 | 1.4680 (19) |
| C15—C16 | 1.394 (4) | O25—S21 | 1.4596 (16) |

| | | | |
|---|---|---|---|
| N1—C2—N3 | 109.0 (2) | C16—C17—H17 | 122.5 |
| N1—C2—N10 | 125.7 (2) | C18—C17—H17 | 120.8 |
| N3—C2—N10 | 125.2 (2) | C17—C18—C19 | 121.7 (2) |
| C5—C4—C9 | 117.5 (2) | C17—C18—N11 | 131.6 (2) |
| C5—C4—H4 | 121.5 | C19—C18—N11 | 106.7 (2) |
| C9—C4—H4 | 121 | C18—C19—C14 | 121.6 (2) |
| C4—C5—C6 | 121.5 (3) | C18—C19—N13 | 106.5 (2) |
| C4—C5—H5 | 119.2 | C14—C19—N13 | 131.8 (2) |
| C6—C5—H5 | 119.3 | C8—N1—C2 | 109.08 (19) |
| C5—C6—C7 | 121.3 (3) | C8—N1—H1 | 127 (2) |
| C5—C6—H6 | 119.3 | C2—N1—H1 | 122 (2) |
| C7—C6—H6 | 119.4 | C9—N3—C2 | 109.2 (2) |
| C6—C7—C8 | 117.2 (3) | C9—N3—H3 | 128.6 (19) |
| C6—C7—H7 | 122 | C2—N3—H3 | 121.9 (19) |
| C8—C7—H7 | 120.8 | H102—N10—C2 | 117 (2) |
| C7—C8—C9 | 121.8 (2) | H102—N10—H101 | 124 (3) |
| C7—C8—N1 | 132.3 (2) | C2—N10—H101 | 117 (2) |
| C9—C8—N1 | 106.0 (2) | C18—N11—C12 | 108.65 (18) |
| C8—C9—C4 | 120.7 (2) | C18—N11—H11 | 125.7 (19) |
| C8—C9—N3 | 106.76 (19) | C12—N11—H11 | 125.5 (19) |
| C4—C9—N3 | 132.5 (2) | C19—N13—C12 | 109.13 (19) |
| N11—C12—N13 | 109.0 (2) | C19—N13—H13 | 125 (2) |
| N11—C12—N20 | 126.2 (2) | C12—N13—H13 | 126 (2) |
| N13—C12—N20 | 124.8 (2) | H202—N20—C12 | 114.7 (18) |
| C15—C14—C19 | 116.6 (2) | H202—N20—H201 | 124 (3) |
| C15—C14—H14 | 122.8 | C12—N20—H201 | 118 (2) |
| C19—C14—H14 | 120.7 | H261—O26—H262 | 100 (6) |
| C14—C15—C16 | 121.6 (3) | O22—S21—O23 | 109.89 (10) |
| C14—C15—H15 | 119.2 | O22—S21—O24 | 108.29 (10) |
| C16—C15—H15 | 119.3 | O23—S21—O24 | 108.23 (12) |
| C15—C16—C17 | 121.7 (3) | O22—S21—O25 | 111.26 (10) |
| C15—C16—H16 | 119.2 | O23—S21—O25 | 108.86 (10) |
| C17—C16—H16 | 119.1 | O24—S21—O25 | 110.26 (13) |
| C16—C17—C18 | 116.8 (2) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O25$^{i}$ | 0.81 (4) | 2.25 (3) | 2.946 (3) | 144 (3) |
| N3—H3···O22$^{ii}$ | 0.83 (3) | 1.93 (3) | 2.749 (3) | 172 (3) |
| N11—H11···O23 | 0.85 (4) | 1.96 (4) | 2.786 (4) | 166 (3) |
| N13—H13···O24$^{iii}$ | 0.83 (4) | 1.91 (4) | 2.720 (3) | 165 (3) |
| N10—H101···O23$^{i}$ | 0.87 (4) | 2.03 (4) | 2.894 (5) | 169 (3) |
| N10—H102···O25$^{ii}$ | 0.89 (3) | 2.00 (3) | 2.890 (3) | 175 (3) |
| N20—H201···O26$^{iii}$ | 0.84 (3) | 2.04 (3) | 2.853 (4) | 165 (3) |
| N20—H202···O22$^{iii}$ | 0.93 (4) | 2.09 (4) | 2.973 (4) | 157 (3) |
| O26—H261···O24$^{iv}$ | 0.80 (7) | 2.22 (7) | 2.983 (4) | 160 (7) |
| O26—H262···O24$^{v}$ | 0.80 (7) | 2.14 (7) | 2.860 (4) | 150 (6) |
| C17—H17···O22 | 0.95 | 2.56 | 3.272 (3) | 132 |

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