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# Crystal structure of *N*-[(4-ethoxyphenyl)carbamothioyl]cyclohexanecarboxamide

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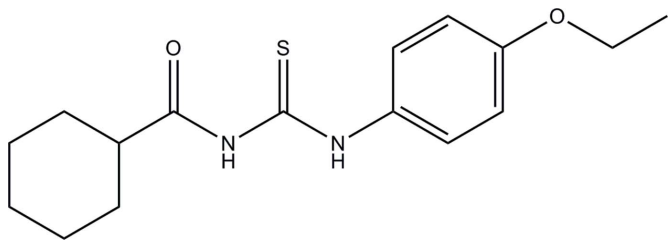
The asymmetric unit of the title compound, $C_{16}H_{22}N_2O_2S$, contains two crystallographically independent molecules (*A* and *B*). In molecule *A*, the cyclohexane ring is disordered over two orientations [occupancy ratio 0.841 (10):0.159 (10)]. In each molecule, the central carbonyl thiourea unit is nearly planar (r.m.s. deviations for all non-H atoms of 0.034 Å in molecule *A* and 0.094 Å in molecule *B*). In both molecules, the cyclohexane ring adopts a chair conformation. The mean plane of the cyclohexane ring makes dihedral angles of 35.8 (4) (molecule *A*) and 20.7 (3)° (molecule *B*) with that of the benzene ring. Each molecule features an intramolecular N—H···O hydrogen bond, which closes an *S*(6) ring motif. In the crystal, molecules are linked *via* pairs of weak N—H···S interactions, forming inversion dimers with an $R_2^2(8)$ ring motif for both molecules. The crystal structure also features weak C—H···$\pi$ ring interactions.

**Keywords:** crystals structure; thiourea derivatives; biological properties; anticorrosion properties; cyclohexanecarboxamide; C—H···$\pi$ interactions.

**CCDC reference**: 1427899

## 1. Related literature

For the biological and anticorrosion properties of thiourea derivatives, see: Hu *et al.* (2011); Sun *et al.* (2006); Shen *et al.* (2006). For related structure see: Vimala *et al.* (2015); Gangadharan *et al.* (2015).



## 2. Experimental

### 2.1. Crystal data

$C_{16}H_{22}N_2O_2S$
$M_r$ = 306.41
Triclinic $P\overline{1}$
$a$ = 10.2273 (7) Å
$b$ = 12.0946 (7) Å
$c$ = 15.2099 (10) Å
$\alpha$ = 70.792 (3)°
$\beta$ = 89.100 (3)°
$\gamma$ = 69.737 (3)°
$V$ = 1656.42 (19) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.20 mm$^{-1}$
$T$ = 293 K
0.30 × 0.20 × 0.20 mm

### 2.2. Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min}$ = 0.942, $T_{max}$ = 0.961
35699 measured reflections
5827 independent reflections
3444 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.049

### 2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.205
$S$ = 1.10
5827 reflections
503 parameters
97 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.38 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.31 e Å$^{-3}$

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

*Cg*1 is the centroid of the C3*A*–C8*A* ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C2*B*—H2*D*···O2*B*$^{i}$ | 0.97 | 2.57 | 3.264 (10) | 128 |
| N1*B*—H3···O2*B* | 0.86 (2) | 1.91 (3) | 2.641 (4) | 142 (4) |
| N1*A*—H1···O2*A* | 0.87 (2) | 1.90 (3) | 2.628 (4) | 140 (4) |
| N2*B*—H4···S1*A*$^{ii}$ | 0.84 (2) | 2.68 (2) | 3.469 (3) | 157 (3) |
| N2*A*—H2···S1*B*$^{iii}$ | 0.85 (2) | 2.73 (3) | 3.430 (3) | 140 (3) |
| C12′—H12*C*···*Cg*1$^{iv}$ | 0.90 | 2.49 (2) | 3.42 (1) | 159 |

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

Data collection: *APEX2* (Bruker, 2008); cell refinement: *APEX2* and *SAINT* (Bruker, 2008); data reduction: *SAINT* and *XPREP* (Bruker, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2009).

## Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: JJ2193).

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# supporting information

*Acta Cryst.* (2015). E**71**, o820–o821 [doi:10.1107/S205698901501806X]

## Crystal structure of *N*-[(4-ethoxyphenyl)carbamothioyl]cyclohexane-carboxamide

**G. Vimala, J. Haribabu, S. Srividya, R. Karvembu and A. SubbiahPandi**

### S1. Comment

The design and synthesis of thioureas are of considerable interest because of their use in agriculture, medicine and analytical chemistry (Hu *et al.*, 2011). Thiourea derivatives are driven by their potential as biological active compounds (Sun *et al.*, 2006) and in material applications such as with their anti corrosion prperties (Shen *et al.*, 2006). In view of their biological importance, the crystal structure of the title compound, $C_{16}H_{22}N_2O_2S$, (I), has been determined herein.

The title compound, (I), contains two crystallographically independent molecules (A and B) in the asymmetric unit (Fig1.). In molecule A, the cyclohexane ring is disordered over two positions [occupancy ratio 0.533 (2): 0.467 (2)]. In each molecule, the central carbonyl thiourea unit is nearly planar (r.m.s. deviations for all non-H atoms of -0.034 Å for C6A and -0.094 Å for C6B. For molecule A, the cyclohexane ring (C11A—C16A) adopts a chairconformation [puckering parameters, q = 0.627 (1) Å, $\theta$ = 6.8°, $\varphi$ = 279 (2)°], while for molecule B, the cyclohexane ring (C11B—C16B) also adopts a chair conformation [puckering, q = 0.546 (6) Å, $\theta$ = 179.3°, $\varphi$ = 219 (2)°;]. The mean plane of the cyclohexane ring makes a dihedral angle of 35.8 (4)° (C3A—C8A) and 20.7 (3)° (C3B—C8B) with that of the benzene ring. Each molecule features an intramolecular N—H···O hydrogen bond (Table 1), which closes an S(6) ring motif. In the crystal, the molecules are linked *via* pairs of N—H···S weak intermolecular interactions, forming inversion dimers with an $R^2_2(8)$ ring motif (Bernstein *et al.* 1995) for both molecules (Fig. 2). The crystal structure is further stabilized by a weak C—H···$\pi$ ring interactions (Table 1).

### S2. Experimental

A mixture of 6-chlorol-3-formylchromone (1 mmol), cyanoacetylindole (1 mmol) and ammonium acetate (1 mmol) in DMF and a catalytic amount of SnCl2.2H2O (0.020 mol %) was added and refluxed for about 3 hrs. After completition of the reaction, the solvent was removed under reduced pressure and the residue was purified by column chromatography on silica gel (3:97% ethylacetate and petether) to afford a pure product. The purified compound was recrystalized from ethanol by using the slow evaporation method. The yield of the isolated product was 92%, giving block-like crystals suitable for *X* ray diffraction.

### S3. Refinement

All H atoms were fixed geometrically and allowed to ride on their parent C atoms, with C—H distances fixed in the range 0.93–0.97 Å with $U_{iso}$(H) = 1.5$U_{eq}$(C) for methyl H atoms and 1.2$U_{eq}$(C) for all other H atoms.

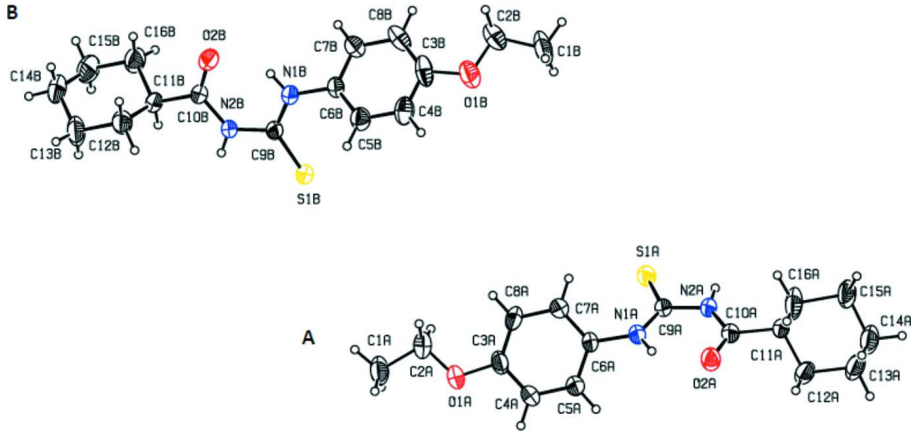


**Figure 1**

The molecular structure of the major component of the title compound, with displacement ellipsoids drawn at 30% probability level.

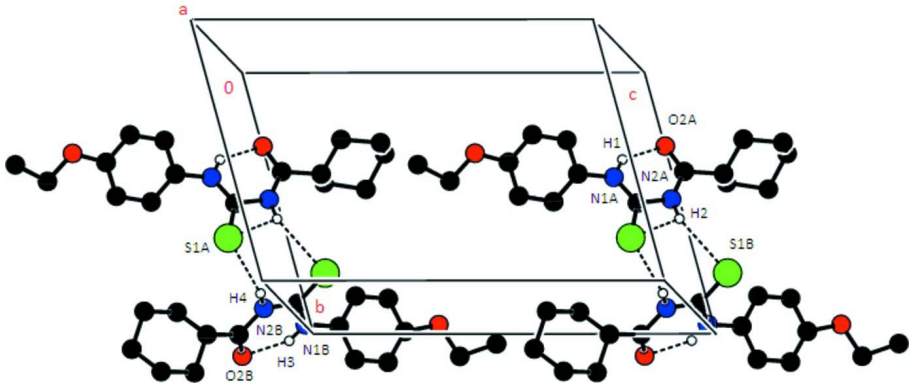


**Figure 2**

A view of the packing of (I) along the *a* axis, showing N—H···O intramolecular hydrogen bonds and molecules linked by weak N—H···S intermolecular interactions along the *b* axis.

### *N*-[(4-Ethoxyphenyl)carbamothioyl]cyclohexanecarboxamide

*Crystal data*

$C_{16}H_{22}N_2O_2S$
$M_r = 306.41$
Triclinic, $P\overline{1}$
$a = 10.2273$ (7) Å
$b = 12.0946$ (7) Å
$c = 15.2099$ (10) Å
$\alpha = 70.792$ (3)°
$\beta = 89.100$ (3)°
$\gamma = 69.737$ (3)°
$V = 1656.42$ (19) Å$^3$
$Z = 4$
$F(000) = 656$
$D_x = 1.229$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3444 reflections
$\theta = 2.3$–25.0°
$\mu = 0.20$ mm$^{-1}$
$T = 293$ K
Block, colourless
0.30 × 0.20 × 0.20 mm

*Data collection*

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Detector resolution: 8.33 pixels mm$^{-1}$
$\omega$ and $\varphi$ scan
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min}$ = 0.942, $T_{max}$ = 0.961
35699 measured reflections
5827 independent reflections
3444 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.049
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 2.3°
$h$ = −12→12
$k$ = −14→14
$l$ = −18→18

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.205
$S$ = 1.10
5827 reflections
503 parameters
97 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0708P)^2 + 1.8566P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.008
$\Delta\rho_{max}$ = 0.38 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.31 e Å$^{-3}$

*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.

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| C3A | 0.6065 (5) | 0.4664 (5) | 0.6568 (3) | 0.0699 (12) | |
| C4A | 0.6435 (5) | 0.3687 (4) | 0.7381 (3) | 0.0724 (12) | |
| H4A | 0.7200 | 0.2965 | 0.7433 | 0.087* | |
| C5A | 0.5696 (4) | 0.3749 (4) | 0.8131 (3) | 0.0641 (11) | |
| H5A | 0.5961 | 0.3065 | 0.8687 | 0.077* | |
| C6A | 0.4571 (4) | 0.4806 (4) | 0.8074 (3) | 0.0538 (9) | |
| C7A | 0.4174 (5) | 0.5790 (4) | 0.7246 (3) | 0.0747 (13) | |
| H7A | 0.3398 | 0.6505 | 0.7191 | 0.090* | |
| C8A | 0.4926 (5) | 0.5725 (5) | 0.6489 (3) | 0.0802 (14) | |
| H8A | 0.4661 | 0.6400 | 0.5927 | 0.096* | |
| C9A | 0.3402 (4) | 0.5683 (3) | 0.9253 (2) | 0.0513 (9) | |
| C10A | 0.2564 (4) | 0.4308 (4) | 1.0544 (3) | 0.0568 (10) | |
| C11A | 0.1943 (6) | 0.4272 (7) | 1.1454 (4) | 0.0594 (14) | 0.841 (10) |
| H11A | 0.1917 | 0.5013 | 1.1595 | 0.071* | 0.841 (10) |
| C12A | 0.2760 (7) | 0.3116 (8) | 1.2256 (4) | 0.091 (2) | 0.841 (10) |
| H12A | 0.3716 | 0.3079 | 1.2331 | 0.109* | 0.841 (10) |
| H12B | 0.2788 | 0.2379 | 1.2120 | 0.109* | 0.841 (10) |
| C13A | 0.2113 (7) | 0.3106 (9) | 1.3156 (4) | 0.102 (2) | 0.841 (10) |
| H13A | 0.2632 | 0.2328 | 1.3655 | 0.122* | 0.841 (10) |
| H13B | 0.2169 | 0.3796 | 1.3327 | 0.122* | 0.841 (10) |

| | | | | | |
|---|---|---|---|---|---|
| C14A | 0.0626 (13) | 0.3229 (14) | 1.3048 (7) | 0.101 (3) | 0.841 (10) |
| H14A | 0.0224 | 0.3236 | 1.3629 | 0.121* | 0.841 (10) |
| H14B | 0.0575 | 0.2513 | 1.2916 | 0.121* | 0.841 (10) |
| C15A | −0.0204 (7) | 0.4420 (9) | 1.2265 (4) | 0.111 (3) | 0.841 (10) |
| H15A | −0.0160 | 0.5146 | 1.2386 | 0.134* | 0.841 (10) |
| H15B | −0.1179 | 0.4502 | 1.2204 | 0.134* | 0.841 (10) |
| C16A | 0.0492 (7) | 0.4315 (11) | 1.1333 (5) | 0.127 (4) | 0.841 (10) |
| H16A | 0.0498 | 0.3560 | 1.1235 | 0.153* | 0.841 (10) |
| H16B | −0.0037 | 0.5035 | 1.0794 | 0.153* | 0.841 (10) |
| C11′ | 0.157 (3) | 0.446 (5) | 1.1254 (18) | 0.0594 (14) | 0.159 (10) |
| H11′ | 0.1460 | 0.5334 | 1.1146 | 0.071* | 0.159 (10) |
| C12′ | 0.249 (3) | 0.394 (4) | 1.2150 (19) | 0.080 (9) | 0.159 (10) |
| H12C | 0.3113 | 0.4397 | 1.2124 | 0.096* | 0.159 (10) |
| H12D | 0.3051 | 0.3061 | 1.2282 | 0.096* | 0.159 (10) |
| C13′ | 0.148 (4) | 0.410 (4) | 1.291 (3) | 0.095 (10) | 0.159 (10) |
| H13C | 0.2041 | 0.3842 | 1.3503 | 0.114* | 0.159 (10) |
| H13D | 0.0920 | 0.4985 | 1.2748 | 0.114* | 0.159 (10) |
| C14′ | 0.049 (6) | 0.337 (5) | 1.306 (3) | 0.072 (9) | 0.159 (10) |
| H14C | 0.1025 | 0.2479 | 1.3339 | 0.087* | 0.159 (10) |
| H14D | −0.0174 | 0.3617 | 1.3485 | 0.087* | 0.159 (10) |
| C15′ | −0.029 (3) | 0.363 (2) | 1.213 (2) | 0.070 (7) | 0.159 (10) |
| H15C | −0.0033 | 0.2885 | 1.1965 | 0.084* | 0.159 (10) |
| H15D | −0.1297 | 0.3958 | 1.2151 | 0.084* | 0.159 (10) |
| C16′ | 0.020 (3) | 0.461 (2) | 1.147 (2) | 0.056 (5) | 0.159 (10) |
| H16C | −0.0363 | 0.4892 | 1.0878 | 0.068* | 0.159 (10) |
| H16D | −0.0100 | 0.5314 | 1.1695 | 0.068* | 0.159 (10) |
| C3B | −0.4223 (6) | 0.9039 (7) | 0.1897 (4) | 0.0888 (16) | |
| C4B | −0.3314 (6) | 0.7967 (5) | 0.1788 (3) | 0.0853 (15) | |
| H4B | −0.3251 | 0.7187 | 0.2209 | 0.102* | |
| C5B | −0.2503 (5) | 0.8033 (4) | 0.1071 (3) | 0.0706 (12) | |
| H5B | −0.1893 | 0.7299 | 0.1000 | 0.085* | |
| C6B | −0.2580 (4) | 0.9180 (4) | 0.0450 (3) | 0.0543 (9) | |
| C7B | −0.3527 (4) | 1.0252 (4) | 0.0530 (3) | 0.0680 (11) | |
| H7B | −0.3611 | 1.1029 | 0.0096 | 0.082* | |
| C8B | −0.4358 (5) | 1.0185 (5) | 0.1255 (4) | 0.0831 (14) | |
| H8B | −0.5007 | 1.0915 | 0.1307 | 0.100* | |
| C9B | −0.0343 (4) | 0.8755 (3) | −0.0218 (2) | 0.0530 (9) | |
| C10B | −0.0317 (5) | 0.9956 (4) | −0.1891 (3) | 0.0596 (10) | |
| C11B | 0.0708 (4) | 1.0160 (4) | −0.2589 (3) | 0.0645 (11) | |
| H11B | 0.1621 | 0.9908 | −0.2238 | 0.077* | |
| C12B | 0.0870 (6) | 0.9341 (4) | −0.3166 (3) | 0.0835 (14) | |
| H12E | −0.0036 | 0.9536 | −0.3488 | 0.100* | |
| H12F | 0.1195 | 0.8470 | −0.2757 | 0.100* | |
| C13B | 0.1893 (7) | 0.9515 (6) | −0.3879 (4) | 0.118 (2) | |
| H13E | 0.2826 | 0.9221 | −0.3559 | 0.142* | |
| H13F | 0.1914 | 0.9017 | −0.4270 | 0.142* | |
| C14B | 0.1479 (7) | 1.0875 (6) | −0.4484 (4) | 0.111 (2) | |
| H14E | 0.2193 | 1.0971 | −0.4899 | 0.133* | |

| | | | | | |
|---|---|---|---|---|---|
| H14F | 0.0605 | 1.1132 | −0.4868 | 0.133* | |
| C15B | 0.1305 (7) | 1.1697 (5) | −0.3922 (4) | 0.1058 (19) | |
| H15E | 0.0968 | 1.2566 | −0.4337 | 0.127* | |
| H15F | 0.2210 | 1.1518 | −0.3607 | 0.127* | |
| C16B | 0.0288 (6) | 1.1527 (4) | −0.3196 (3) | 0.0879 (15) | |
| H16E | 0.0279 | 1.2023 | −0.2806 | 0.106* | |
| H16F | −0.0651 | 1.1823 | −0.3508 | 0.106* | |
| N1A | 0.3837 (3) | 0.4788 (3) | 0.8879 (2) | 0.0570 (8) | |
| N2A | 0.2747 (3) | 0.5405 (3) | 1.0059 (2) | 0.0529 (8) | |
| N1B | −0.1730 (3) | 0.9287 (3) | −0.0299 (2) | 0.0571 (8) | |
| N2B | 0.0275 (4) | 0.9065 (3) | −0.1033 (2) | 0.0576 (9) | |
| O2A | 0.2912 (3) | 0.3411 (3) | 1.0280 (2) | 0.0735 (8) | |
| O2B | −0.1578 (3) | 1.0514 (3) | −0.20668 (19) | 0.0787 (9) | |
| S1A | 0.36072 (12) | 0.70593 (10) | 0.88640 (8) | 0.0664 (3) | |
| S1B | 0.06988 (12) | 0.78100 (10) | 0.07648 (7) | 0.0643 (3) | |
| C1A | 0.7842 (10) | 0.5119 (10) | 0.4461 (6) | 0.102 (3) | 0.867 (13) |
| H1A | 0.8710 | 0.5065 | 0.4736 | 0.153* | 0.867 (13) |
| H1B | 0.7622 | 0.5724 | 0.3838 | 0.153* | 0.867 (13) |
| H1C | 0.7928 | 0.4313 | 0.4439 | 0.153* | 0.867 (13) |
| C2A | 0.6698 (8) | 0.5516 (6) | 0.5040 (4) | 0.087 (2) | 0.867 (13) |
| H2A | 0.6723 | 0.6239 | 0.5174 | 0.104* | 0.867 (13) |
| H2B | 0.5790 | 0.5741 | 0.4707 | 0.104* | 0.867 (13) |
| O1A | 0.6919 (7) | 0.4496 (5) | 0.5875 (3) | 0.089 (2) | 0.867 (13) |
| C1A′ | 0.800 (13) | 0.453 (7) | 0.457 (6) | 0.24 (7) | 0.133 (13) |
| H1′1 | 0.8898 | 0.3905 | 0.4595 | 0.354* | 0.133 (13) |
| H1′2 | 0.7327 | 0.4499 | 0.4161 | 0.354* | 0.133 (13) |
| H1′3 | 0.8071 | 0.5348 | 0.4351 | 0.354* | 0.133 (13) |
| C2A′ | 0.754 (4) | 0.429 (5) | 0.554 (4) | 0.12 (2) | 0.133 (13) |
| H2′1 | 0.7514 | 0.3448 | 0.5758 | 0.141* | 0.133 (13) |
| H2′2 | 0.8256 | 0.4294 | 0.5947 | 0.141* | 0.133 (13) |
| O1A′ | 0.625 (3) | 0.512 (4) | 0.5633 (14) | 0.113 (19) | 0.133 (13) |
| C1B | −0.608 (2) | 0.913 (3) | 0.3917 (12) | 0.162 (10) | 0.705 (13) |
| H1D | −0.6418 | 0.8479 | 0.3911 | 0.243* | 0.705 (13) |
| H1E | −0.6811 | 0.9766 | 0.4070 | 0.243* | 0.705 (13) |
| H1F | −0.5282 | 0.8774 | 0.4377 | 0.243* | 0.705 (13) |
| C2B | −0.5672 (9) | 0.9695 (9) | 0.2959 (8) | 0.096 (3) | 0.705 (13) |
| H2D | −0.6494 | 1.0189 | 0.2505 | 0.115* | 0.705 (13) |
| H2E | −0.5159 | 1.0228 | 0.2981 | 0.115* | 0.705 (13) |
| O1B | −0.4816 (6) | 0.8658 (7) | 0.2729 (5) | 0.094 (2) | 0.705 (13) |
| O1B′ | −0.5264 (13) | 0.9542 (12) | 0.2458 (8) | 0.077 (5) | 0.295 (13) |
| C1B′ | −0.622 (3) | 0.897 (6) | 0.391 (2) | 0.094 (12) | 0.295 (13) |
| H1G | −0.7127 | 0.8934 | 0.3821 | 0.141* | 0.295 (13) |
| H1H | −0.6312 | 0.9823 | 0.3809 | 0.141* | 0.295 (13) |
| H1I | −0.5803 | 0.8455 | 0.4542 | 0.141* | 0.295 (13) |
| C2B′ | −0.530 (2) | 0.8499 (16) | 0.3233 (12) | 0.076 (6) | 0.295 (13) |
| H2F | −0.4355 | 0.7989 | 0.3542 | 0.091* | 0.295 (13) |
| H2G | −0.5661 | 0.7982 | 0.3015 | 0.091* | 0.295 (13) |
| H3 | −0.208 (4) | 0.983 (3) | −0.0843 (17) | 0.064 (12)* | |

| | | | | |
|---|---|---|---|---|
| H1 | 0.373 (4) | 0.409 (2) | 0.920 (3) | 0.069 (13)* |
| H4 | 0.115 (2) | 0.868 (3) | −0.094 (2) | 0.052 (11)* |
| H2 | 0.259 (7) | 0.612 (3) | 1.011 (4) | 0.18 (3)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C3A | 0.073 (3) | 0.086 (3) | 0.056 (3) | −0.026 (3) | 0.024 (2) | −0.036 (2) |
| C4A | 0.069 (3) | 0.072 (3) | 0.065 (3) | −0.008 (2) | 0.021 (2) | −0.028 (2) |
| C5A | 0.072 (3) | 0.057 (2) | 0.057 (2) | −0.016 (2) | 0.017 (2) | −0.019 (2) |
| C6A | 0.060 (2) | 0.059 (2) | 0.043 (2) | −0.0187 (19) | 0.0148 (18) | −0.0212 (18) |
| C7A | 0.076 (3) | 0.071 (3) | 0.055 (3) | −0.002 (2) | 0.012 (2) | −0.020 (2) |
| C8A | 0.107 (4) | 0.083 (3) | 0.040 (2) | −0.029 (3) | 0.015 (2) | −0.013 (2) |
| C9A | 0.048 (2) | 0.054 (2) | 0.044 (2) | −0.0123 (17) | 0.0081 (17) | −0.0143 (17) |
| C10A | 0.062 (2) | 0.053 (2) | 0.051 (2) | −0.0176 (19) | 0.0136 (19) | −0.0161 (19) |
| C11A | 0.070 (3) | 0.053 (3) | 0.044 (3) | −0.015 (3) | 0.017 (2) | −0.011 (3) |
| C12A | 0.078 (3) | 0.099 (4) | 0.058 (3) | −0.018 (3) | 0.013 (2) | 0.005 (3) |
| C13A | 0.099 (4) | 0.122 (6) | 0.054 (3) | −0.036 (4) | 0.016 (3) | 0.003 (3) |
| C14A | 0.105 (5) | 0.134 (7) | 0.057 (4) | −0.051 (4) | 0.029 (3) | −0.019 (3) |
| C15A | 0.076 (4) | 0.164 (7) | 0.063 (3) | −0.033 (4) | 0.033 (3) | −0.012 (3) |
| C16A | 0.064 (4) | 0.242 (10) | 0.049 (3) | −0.045 (4) | 0.019 (3) | −0.029 (4) |
| C11′ | 0.070 (3) | 0.053 (3) | 0.044 (3) | −0.015 (3) | 0.017 (2) | −0.011 (3) |
| C12′ | 0.084 (9) | 0.10 (2) | 0.045 (5) | −0.045 (9) | 0.011 (5) | 0.000 (7) |
| C13′ | 0.124 (14) | 0.13 (2) | 0.074 (10) | −0.095 (16) | 0.046 (10) | −0.039 (12) |
| C14′ | 0.073 (15) | 0.063 (18) | 0.087 (12) | −0.038 (14) | 0.032 (9) | −0.020 (9) |
| C15′ | 0.068 (12) | 0.044 (11) | 0.093 (12) | −0.014 (9) | 0.024 (8) | −0.024 (9) |
| C16′ | 0.070 (5) | 0.037 (9) | 0.071 (12) | −0.014 (5) | 0.024 (5) | −0.036 (8) |
| C3B | 0.083 (3) | 0.147 (5) | 0.078 (3) | −0.071 (4) | 0.045 (3) | −0.062 (4) |
| C4B | 0.097 (4) | 0.106 (4) | 0.070 (3) | −0.061 (3) | 0.033 (3) | −0.027 (3) |
| C5B | 0.082 (3) | 0.070 (3) | 0.067 (3) | −0.035 (2) | 0.021 (2) | −0.026 (2) |
| C6B | 0.059 (2) | 0.061 (2) | 0.047 (2) | −0.0248 (19) | 0.0162 (18) | −0.0217 (19) |
| C7B | 0.062 (3) | 0.071 (3) | 0.074 (3) | −0.021 (2) | 0.018 (2) | −0.032 (2) |
| C8B | 0.061 (3) | 0.107 (4) | 0.105 (4) | −0.030 (3) | 0.032 (3) | −0.067 (3) |
| C9B | 0.066 (3) | 0.046 (2) | 0.045 (2) | −0.0159 (18) | 0.0125 (18) | −0.0172 (17) |
| C10B | 0.066 (3) | 0.057 (2) | 0.043 (2) | −0.012 (2) | 0.0104 (19) | −0.0114 (18) |
| C11B | 0.065 (3) | 0.070 (3) | 0.042 (2) | −0.014 (2) | 0.0096 (19) | −0.0082 (19) |
| C12B | 0.102 (4) | 0.074 (3) | 0.071 (3) | −0.031 (3) | 0.030 (3) | −0.024 (3) |
| C13B | 0.166 (6) | 0.111 (4) | 0.080 (4) | −0.051 (4) | 0.069 (4) | −0.038 (3) |
| C14B | 0.143 (5) | 0.117 (5) | 0.058 (3) | −0.045 (4) | 0.038 (3) | −0.014 (3) |
| C15B | 0.129 (5) | 0.094 (4) | 0.087 (4) | −0.057 (4) | 0.037 (4) | −0.006 (3) |
| C16B | 0.118 (4) | 0.076 (3) | 0.072 (3) | −0.043 (3) | 0.027 (3) | −0.020 (3) |
| N1A | 0.065 (2) | 0.053 (2) | 0.0495 (19) | −0.0166 (17) | 0.0179 (16) | −0.0186 (16) |
| N2A | 0.0588 (19) | 0.0508 (19) | 0.0436 (17) | −0.0186 (15) | 0.0152 (15) | −0.0112 (15) |
| N1B | 0.056 (2) | 0.062 (2) | 0.0442 (19) | −0.0158 (17) | 0.0111 (16) | −0.0128 (16) |
| N2B | 0.057 (2) | 0.0558 (19) | 0.0431 (18) | −0.0065 (16) | 0.0137 (16) | −0.0110 (15) |
| O2A | 0.102 (2) | 0.0593 (17) | 0.0655 (18) | −0.0327 (16) | 0.0270 (17) | −0.0270 (15) |
| O2B | 0.069 (2) | 0.090 (2) | 0.0521 (17) | −0.0147 (17) | 0.0034 (15) | −0.0073 (15) |
| S1A | 0.0728 (7) | 0.0585 (6) | 0.0632 (7) | −0.0220 (5) | 0.0257 (5) | −0.0177 (5) |

| | | | | | | |
|---|---|---|---|---|---|---|
| S1B | 0.0715 (7) | 0.0613 (6) | 0.0449 (6) | −0.0107 (5) | 0.0108 (5) | −0.0137 (5) |
| C1A | 0.116 (6) | 0.122 (8) | 0.074 (4) | −0.049 (5) | 0.048 (4) | −0.038 (5) |
| C2A | 0.105 (5) | 0.108 (5) | 0.055 (4) | −0.043 (4) | 0.026 (4) | −0.033 (3) |
| O1A | 0.089 (6) | 0.097 (4) | 0.063 (3) | −0.015 (4) | 0.035 (3) | −0.028 (3) |
| C1A′ | 0.37 (14) | 0.12 (7) | 0.25 (10) | −0.10 (7) | 0.26 (10) | −0.10 (7) |
| C2A′ | 0.07 (3) | 0.13 (5) | 0.18 (7) | −0.02 (3) | 0.02 (3) | −0.09 (5) |
| O1A′ | 0.045 (19) | 0.21 (5) | 0.08 (3) | −0.02 (2) | 0.023 (16) | −0.07 (3) |
| C1B | 0.198 (18) | 0.169 (17) | 0.119 (15) | −0.052 (15) | 0.111 (12) | −0.069 (13) |
| C2B | 0.073 (5) | 0.119 (8) | 0.111 (8) | −0.030 (5) | 0.037 (5) | −0.064 (7) |
| O1B | 0.096 (4) | 0.102 (5) | 0.099 (6) | −0.044 (4) | 0.051 (4) | −0.049 (5) |
| O1B′ | 0.082 (9) | 0.060 (8) | 0.080 (9) | −0.018 (7) | 0.049 (7) | −0.024 (7) |
| C1B′ | 0.046 (12) | 0.14 (3) | 0.07 (2) | −0.018 (15) | 0.013 (12) | −0.027 (18) |
| C2B′ | 0.065 (12) | 0.089 (14) | 0.069 (12) | −0.032 (10) | 0.020 (9) | −0.019 (10) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C3A—C4A | 1.346 (6) | C5B—H5B | 0.9300 |
| C3A—C8A | 1.373 (6) | C6B—C7B | 1.366 (5) |
| C3A—O1A | 1.381 (6) | C6B—N1B | 1.421 (5) |
| C3A—O1A′ | 1.383 (19) | C7B—C8B | 1.379 (6) |
| C4A—C5A | 1.366 (5) | C7B—H7B | 0.9300 |
| C4A—H4A | 0.9300 | C8B—H8B | 0.9300 |
| C5A—C6A | 1.370 (5) | C9B—N1B | 1.328 (5) |
| C5A—H5A | 0.9300 | C9B—N2B | 1.382 (5) |
| C6A—C7A | 1.364 (5) | C9B—S1B | 1.661 (4) |
| C6A—N1A | 1.423 (5) | C10B—O2B | 1.217 (5) |
| C7A—C8A | 1.384 (6) | C10B—N2B | 1.371 (5) |
| C7A—H7A | 0.9300 | C10B—C11B | 1.502 (5) |
| C8A—H8A | 0.9300 | C11B—C12B | 1.494 (6) |
| C9A—N1A | 1.326 (5) | C11B—C16B | 1.512 (6) |
| C9A—N2A | 1.387 (4) | C11B—H11B | 0.9800 |
| C9A—S1A | 1.659 (4) | C12B—C13B | 1.510 (6) |
| C10A—O2A | 1.216 (4) | C12B—H12E | 0.9700 |
| C10A—N2A | 1.366 (5) | C12B—H12F | 0.9700 |
| C10A—C11′ | 1.482 (17) | C13B—C14B | 1.505 (7) |
| C10A—C11A | 1.508 (6) | C13B—H13E | 0.9700 |
| C11A—C16A | 1.479 (8) | C13B—H13F | 0.9700 |
| C11A—C12A | 1.497 (7) | C14B—C15B | 1.479 (8) |
| C11A—H11A | 0.9800 | C14B—H14E | 0.9700 |
| C12A—C13A | 1.510 (7) | C14B—H14F | 0.9700 |
| C12A—H12A | 0.9700 | C15B—C16B | 1.519 (7) |
| C12A—H12B | 0.9700 | C15B—H15E | 0.9700 |
| C13A—C14A | 1.482 (11) | C15B—H15F | 0.9700 |
| C13A—H13A | 0.9700 | C16B—H16E | 0.9700 |
| C13A—H13B | 0.9700 | C16B—H16F | 0.9700 |
| C14A—C15A | 1.506 (12) | N1A—H1 | 0.871 (19) |
| C14A—H14A | 0.9700 | N2A—H2 | 0.85 (2) |
| C14A—H14B | 0.9700 | N1B—H3 | 0.855 (19) |

| | | | |
|---|---|---|---|
| C15A—C16A | 1.599 (9) | N2B—H4 | 0.841 (18) |
| C15A—H15A | 0.9700 | C1A—C2A | 1.493 (9) |
| C15A—H15B | 0.9700 | C1A—H1A | 0.9600 |
| C16A—H16A | 0.9700 | C1A—H1B | 0.9600 |
| C16A—H16B | 0.9700 | C1A—H1C | 0.9600 |
| C11′—C16′ | 1.402 (18) | C2A—O1A | 1.404 (7) |
| C11′—C12′ | 1.485 (19) | C2A—H2A | 0.9700 |
| C11′—H11′ | 0.9800 | C2A—H2B | 0.9700 |
| C12′—C13′ | 1.555 (19) | C1A′—C2A′ | 1.49 (2) |
| C12′—H12C | 0.9700 | C1A′—H1′1 | 0.9600 |
| C12′—H12D | 0.9700 | C1A′—H1′2 | 0.9600 |
| C13′—C14′ | 1.53 (2) | C1A′—H1′3 | 0.9600 |
| C13′—H13C | 0.9700 | C2A′—O1A′ | 1.40 (2) |
| C13′—H13D | 0.9700 | C2A′—H2′1 | 0.9700 |
| C14′—C15′ | 1.51 (2) | C2A′—H2′2 | 0.9700 |
| C14′—H14C | 0.9700 | C1B—C2B | 1.515 (17) |
| C14′—H14D | 0.9700 | C1B—H1D | 0.9600 |
| C15′—C16′ | 1.505 (19) | C1B—H1E | 0.9600 |
| C15′—H15C | 0.9700 | C1B—H1F | 0.9600 |
| C15′—H15D | 0.9700 | C2B—O1B | 1.408 (9) |
| C16′—H16C | 0.9700 | C2B—H2D | 0.9700 |
| C16′—H16D | 0.9700 | C2B—H2E | 0.9700 |
| C3B—C4B | 1.369 (7) | O1B′—C2B′ | 1.426 (15) |
| C3B—C8B | 1.370 (7) | C1B′—C2B′ | 1.51 (2) |
| C3B—O1B | 1.403 (7) | C1B′—H1G | 0.9600 |
| C3B—O1B′ | 1.448 (12) | C1B′—H1H | 0.9600 |
| C4B—C5B | 1.358 (6) | C1B′—H1I | 0.9600 |
| C4B—H4B | 0.9300 | C2B′—H2F | 0.9700 |
| C5B—C6B | 1.373 (5) | C2B′—H2G | 0.9700 |

| | | | |
|---|---|---|---|
| C4A—C3A—C8A | 119.7 (4) | C5B—C6B—N1B | 121.8 (4) |
| C4A—C3A—O1A | 114.8 (4) | C6B—C7B—C8B | 120.2 (4) |
| C8A—C3A—O1A | 125.5 (5) | C6B—C7B—H7B | 119.9 |
| C4A—C3A—O1A′ | 147.5 (17) | C8B—C7B—H7B | 119.9 |
| C8A—C3A—O1A′ | 92.4 (16) | C3B—C8B—C7B | 119.7 (5) |
| C3A—C4A—C5A | 120.5 (4) | C3B—C8B—H8B | 120.2 |
| C3A—C4A—H4A | 119.7 | C7B—C8B—H8B | 120.2 |
| C5A—C4A—H4A | 119.7 | N1B—C9B—N2B | 115.7 (3) |
| C4A—C5A—C6A | 120.9 (4) | N1B—C9B—S1B | 126.3 (3) |
| C4A—C5A—H5A | 119.6 | N2B—C9B—S1B | 117.9 (3) |
| C6A—C5A—H5A | 119.6 | O2B—C10B—N2B | 121.7 (4) |
| C7A—C6A—C5A | 118.8 (4) | O2B—C10B—C11B | 123.5 (3) |
| C7A—C6A—N1A | 123.6 (3) | N2B—C10B—C11B | 114.7 (4) |
| C5A—C6A—N1A | 117.5 (3) | C12B—C11B—C10B | 110.1 (4) |
| C6A—C7A—C8A | 120.1 (4) | C12B—C11B—C16B | 111.5 (4) |
| C6A—C7A—H7A | 119.9 | C10B—C11B—C16B | 111.7 (4) |
| C8A—C7A—H7A | 119.9 | C12B—C11B—H11B | 107.8 |
| C3A—C8A—C7A | 119.9 (4) | C10B—C11B—H11B | 107.8 |

| | | | |
|---|---|---|---|
| C3A—C8A—H8A | 120.1 | C16B—C11B—H11B | 107.8 |
| C7A—C8A—H8A | 120.1 | C11B—C12B—C13B | 112.0 (4) |
| N1A—C9A—N2A | 115.5 (3) | C11B—C12B—H12E | 109.2 |
| N1A—C9A—S1A | 126.3 (3) | C13B—C12B—H12E | 109.2 |
| N2A—C9A—S1A | 118.2 (3) | C11B—C12B—H12F | 109.2 |
| O2A—C10A—N2A | 122.9 (4) | C13B—C12B—H12F | 109.2 |
| O2A—C10A—C11′ | 123 (2) | H12E—C12B—H12F | 107.9 |
| N2A—C10A—C11′ | 112 (2) | C14B—C13B—C12B | 110.8 (5) |
| O2A—C10A—C11A | 122.2 (4) | C14B—C13B—H13E | 109.5 |
| N2A—C10A—C11A | 114.9 (4) | C12B—C13B—H13E | 109.5 |
| C16A—C11A—C12A | 109.2 (6) | C14B—C13B—H13F | 109.5 |
| C16A—C11A—C10A | 108.1 (5) | C12B—C13B—H13F | 109.5 |
| C12A—C11A—C10A | 112.5 (5) | H13E—C13B—H13F | 108.1 |
| C16A—C11A—H11A | 109.0 | C15B—C14B—C13B | 112.1 (5) |
| C12A—C11A—H11A | 109.0 | C15B—C14B—H14E | 109.2 |
| C10A—C11A—H11A | 109.0 | C13B—C14B—H14E | 109.2 |
| C11A—C12A—C13A | 111.3 (5) | C15B—C14B—H14F | 109.2 |
| C11A—C12A—H12A | 109.4 | C13B—C14B—H14F | 109.2 |
| C13A—C12A—H12A | 109.4 | H14E—C14B—H14F | 107.9 |
| C11A—C12A—H12B | 109.4 | C14B—C15B—C16B | 112.7 (5) |
| C13A—C12A—H12B | 109.4 | C14B—C15B—H15E | 109.1 |
| H12A—C12A—H12B | 108.0 | C16B—C15B—H15E | 109.1 |
| C14A—C13A—C12A | 110.6 (7) | C14B—C15B—H15F | 109.1 |
| C14A—C13A—H13A | 109.5 | C16B—C15B—H15F | 109.1 |
| C12A—C13A—H13A | 109.5 | H15E—C15B—H15F | 107.8 |
| C14A—C13A—H13B | 109.5 | C11B—C16B—C15B | 110.6 (4) |
| C12A—C13A—H13B | 109.5 | C11B—C16B—H16E | 109.5 |
| H13A—C13A—H13B | 108.1 | C15B—C16B—H16E | 109.5 |
| C13A—C14A—C15A | 110.8 (7) | C11B—C16B—H16F | 109.5 |
| C13A—C14A—H14A | 109.5 | C15B—C16B—H16F | 109.5 |
| C15A—C14A—H14A | 109.5 | H16E—C16B—H16F | 108.1 |
| C13A—C14A—H14B | 109.5 | C9A—N1A—C6A | 127.3 (3) |
| C15A—C14A—H14B | 109.5 | C9A—N1A—H1 | 115 (3) |
| H14A—C14A—H14B | 108.1 | C6A—N1A—H1 | 118 (3) |
| C14A—C15A—C16A | 106.3 (10) | C10A—N2A—C9A | 128.4 (3) |
| C14A—C15A—H15A | 110.5 | C10A—N2A—H2 | 138 (3) |
| C16A—C15A—H15A | 110.5 | C9A—N2A—H2 | 93 (2) |
| C14A—C15A—H15B | 110.5 | C9B—N1B—C6B | 125.7 (3) |
| C16A—C15A—H15B | 110.5 | C9B—N1B—H3 | 113 (3) |
| H15A—C15A—H15B | 108.7 | C6B—N1B—H3 | 120 (3) |
| C11A—C16A—C15A | 107.4 (7) | C10B—N2B—C9B | 129.1 (3) |
| C11A—C16A—H16A | 110.2 | C10B—N2B—H4 | 119 (3) |
| C15A—C16A—H16A | 110.2 | C9B—N2B—H4 | 112 (3) |
| C11A—C16A—H16B | 110.2 | C2A—C1A—H1A | 109.5 |
| C15A—C16A—H16B | 110.2 | C2A—C1A—H1B | 109.5 |
| H16A—C16A—H16B | 108.5 | H1A—C1A—H1B | 109.5 |
| C16′—C11′—C10A | 146 (3) | C2A—C1A—H1C | 109.5 |
| C16′—C11′—C12′ | 108 (2) | H1A—C1A—H1C | 109.5 |

| | | | |
|---|---|---|---|
| C10A—C11′—C12′ | 104.1 (17) | H1B—C1A—H1C | 109.5 |
| C16′—C11′—H11′ | 94.8 | O1A—C2A—C1A | 107.2 (7) |
| C10A—C11′—H11′ | 94.8 | O1A—C2A—H2A | 110.3 |
| C12′—C11′—H11′ | 94.8 | C1A—C2A—H2A | 110.3 |
| C11′—C12′—C13′ | 106 (2) | O1A—C2A—H2B | 110.3 |
| C11′—C12′—H12C | 110.6 | C1A—C2A—H2B | 110.3 |
| C13′—C12′—H12C | 110.6 | H2A—C2A—H2B | 108.5 |
| C11′—C12′—H12D | 110.6 | C3A—O1A—C2A | 118.4 (6) |
| C13′—C12′—H12D | 110.6 | C2A′—C1A′—H1′1 | 109.5 |
| H12C—C12′—H12D | 108.8 | C2A′—C1A′—H1′2 | 109.5 |
| C14′—C13′—C12′ | 116 (4) | H1′1—C1A′—H1′2 | 109.5 |
| C14′—C13′—H13C | 108.3 | C2A′—C1A′—H1′3 | 109.5 |
| C12′—C13′—H13C | 108.3 | H1′1—C1A′—H1′3 | 109.5 |
| C14′—C13′—H13D | 108.3 | H1′2—C1A′—H1′3 | 109.5 |
| C12′—C13′—H13D | 108.3 | O1A′—C2A′—C1A′ | 117 (5) |
| H13C—C13′—H13D | 107.4 | O1A′—C2A′—H2′1 | 108.1 |
| C15′—C14′—C13′ | 110 (3) | C1A′—C2A′—H2′1 | 108.0 |
| C15′—C14′—H14C | 109.6 | O1A′—C2A′—H2′2 | 108.0 |
| C13′—C14′—H14C | 109.6 | C1A′—C2A′—H2′2 | 108.1 |
| C15′—C14′—H14D | 109.6 | H2′1—C2A′—H2′2 | 107.3 |
| C13′—C14′—H14D | 109.6 | C3A—O1A′—C2A′ | 105 (4) |
| H14C—C14′—H14D | 108.1 | C2B—C1B—H1D | 109.5 |
| C16′—C15′—C14′ | 102 (3) | C2B—C1B—H1E | 109.5 |
| C16′—C15′—H15C | 111.4 | H1D—C1B—H1E | 109.5 |
| C14′—C15′—H15C | 111.4 | C2B—C1B—H1F | 109.5 |
| C16′—C15′—H15D | 111.4 | H1D—C1B—H1F | 109.5 |
| C14′—C15′—H15D | 111.4 | H1E—C1B—H1F | 109.5 |
| H15C—C15′—H15D | 109.2 | O1B—C2B—C1B | 104.7 (14) |
| C11′—C16′—C15′ | 127 (3) | O1B—C2B—H2D | 110.8 |
| C11′—C16′—H16C | 105.6 | C1B—C2B—H2D | 110.8 |
| C15′—C16′—H16C | 105.6 | O1B—C2B—H2E | 110.8 |
| C11′—C16′—H16D | 105.6 | C1B—C2B—H2E | 110.8 |
| C15′—C16′—H16D | 105.5 | H2D—C2B—H2E | 108.9 |
| H16C—C16′—H16D | 106.1 | C3B—O1B—C2B | 111.4 (8) |
| C4B—C3B—C8B | 119.7 (4) | C2B′—O1B′—C3B | 106.7 (14) |
| C4B—C3B—O1B | 106.5 (6) | C2B′—C1B′—H1G | 109.5 |
| C8B—C3B—O1B | 133.8 (6) | C2B′—C1B′—H1H | 109.5 |
| C4B—C3B—O1B′ | 145.2 (7) | H1G—C1B′—H1H | 109.5 |
| C8B—C3B—O1B′ | 95.1 (6) | C2B′—C1B′—H1I | 109.5 |
| C5B—C4B—C3B | 120.5 (5) | H1G—C1B′—H1I | 109.5 |
| C5B—C4B—H4B | 119.7 | H1H—C1B′—H1I | 109.5 |
| C3B—C4B—H4B | 119.7 | O1B′—C2B′—C1B′ | 109 (3) |
| C4B—C5B—C6B | 120.2 (4) | O1B′—C2B′—H2F | 109.8 |
| C4B—C5B—H5B | 119.9 | C1B′—C2B′—H2F | 109.8 |
| C6B—C5B—H5B | 119.9 | O1B′—C2B′—H2G | 109.8 |
| C7B—C6B—C5B | 119.6 (4) | C1B′—C2B′—H2G | 109.8 |
| C7B—C6B—N1B | 118.5 (4) | H2F—C2B′—H2G | 108.3 |

| | | | |
|---|---|---|---|
| C8A—C3A—C4A—C5A | −0.7 (7) | O1B—C3B—C8B—C7B | 174.8 (6) |
| O1A—C3A—C4A—C5A | 178.3 (5) | O1B′—C3B—C8B—C7B | 178.5 (7) |
| O1A′—C3A—C4A—C5A | −171 (4) | C6B—C7B—C8B—C3B | 0.5 (7) |
| C3A—C4A—C5A—C6A | −0.4 (7) | O2B—C10B—C11B—C12B | −86.4 (5) |
| C4A—C5A—C6A—C7A | 1.6 (7) | N2B—C10B—C11B—C12B | 92.4 (5) |
| C4A—C5A—C6A—N1A | 178.7 (4) | O2B—C10B—C11B—C16B | 38.1 (6) |
| C5A—C6A—C7A—C8A | −1.7 (7) | N2B—C10B—C11B—C16B | −143.2 (4) |
| N1A—C6A—C7A—C8A | −178.6 (4) | C10B—C11B—C12B—C13B | 180.0 (4) |
| C4A—C3A—C8A—C7A | 0.6 (8) | C16B—C11B—C12B—C13B | 55.4 (6) |
| O1A—C3A—C8A—C7A | −178.2 (5) | C11B—C12B—C13B—C14B | −54.8 (7) |
| O1A′—C3A—C8A—C7A | 175 (2) | C12B—C13B—C14B—C15B | 54.1 (8) |
| C6A—C7A—C8A—C3A | 0.6 (8) | C13B—C14B—C15B—C16B | −54.3 (7) |
| O2A—C10A—C11A—C16A | −73.2 (7) | C12B—C11B—C16B—C15B | −53.8 (6) |
| N2A—C10A—C11A—C16A | 108.9 (7) | C10B—C11B—C16B—C15B | −177.5 (4) |
| O2A—C10A—C11A—C12A | 47.5 (8) | C14B—C15B—C16B—C11B | 53.7 (7) |
| N2A—C10A—C11A—C12A | −130.4 (6) | N2A—C9A—N1A—C6A | −178.0 (3) |
| C16A—C11A—C12A—C13A | −59.9 (9) | S1A—C9A—N1A—C6A | 0.3 (6) |
| C10A—C11A—C12A—C13A | −180.0 (6) | C7A—C6A—N1A—C9A | −47.9 (6) |
| C11A—C12A—C13A—C14A | 56.1 (10) | C5A—C6A—N1A—C9A | 135.1 (4) |
| C12A—C13A—C14A—C15A | −58.2 (13) | O2A—C10A—N2A—C9A | −4.3 (7) |
| C13A—C14A—C15A—C16A | 61.0 (13) | C11′—C10A—N2A—C9A | −168.6 (14) |
| C12A—C11A—C16A—C15A | 63.0 (11) | C11A—C10A—N2A—C9A | 173.6 (4) |
| C10A—C11A—C16A—C15A | −174.2 (8) | N1A—C9A—N2A—C10A | 4.1 (6) |
| C14A—C15A—C16A—C11A | −63.5 (11) | S1A—C9A—N2A—C10A | −174.4 (3) |
| O2A—C10A—C11′—C16′ | −63 (7) | N2B—C9B—N1B—C6B | −175.4 (3) |
| N2A—C10A—C11′—C16′ | 101 (7) | S1B—C9B—N1B—C6B | 2.4 (6) |
| O2A—C10A—C11′—C12′ | 95 (3) | C7B—C6B—N1B—C9B | 128.5 (4) |
| N2A—C10A—C11′—C12′ | −101 (3) | C5B—C6B—N1B—C9B | −53.5 (6) |
| C16′—C11′—C12′—C13′ | −14 (5) | O2B—C10B—N2B—C9B | −9.1 (7) |
| C10A—C11′—C12′—C13′ | 179 (3) | C11B—C10B—N2B—C9B | 172.1 (4) |
| C11′—C12′—C13′—C14′ | 63 (5) | N1B—C9B—N2B—C10B | 8.7 (6) |
| C12′—C13′—C14′—C15′ | −52 (6) | S1B—C9B—N2B—C10B | −169.2 (3) |
| C13′—C14′—C15′—C16′ | −4 (5) | C4A—C3A—O1A—C2A | −173.4 (6) |
| C10A—C11′—C16′—C15′ | 105 (7) | C8A—C3A—O1A—C2A | 5.5 (10) |
| C12′—C11′—C16′—C15′ | −52 (6) | C1A—C2A—O1A—C3A | 174.4 (6) |
| C14′—C15′—C16′—C11′ | 63 (5) | C4A—C3A—O1A′—C2A′ | −19 (7) |
| C8B—C3B—C4B—C5B | 2.8 (8) | C8A—C3A—O1A′—C2A′ | 170 (4) |
| O1B—C3B—C4B—C5B | −175.7 (5) | C1A′—C2A′—O1A′—C3A | 178 (6) |
| O1B′—C3B—C4B—C5B | 179.8 (12) | C4B—C3B—O1B—C2B | 174.2 (6) |
| C3B—C4B—C5B—C6B | 0.5 (7) | C8B—C3B—O1B—C2B | −4.0 (10) |
| C4B—C5B—C6B—C7B | −3.2 (7) | C1B—C2B—O1B—C3B | −173.5 (11) |
| C4B—C5B—C6B—N1B | 178.8 (4) | C4B—C3B—O1B′—C2B′ | 5 (2) |
| C5B—C6B—C7B—C8B | 2.7 (7) | C8B—C3B—O1B′—C2B′ | −177.8 (11) |
| N1B—C6B—C7B—C8B | −179.2 (4) | C3B—O1B′—C2B′—C1B′ | 172.4 (19) |
| C4B—C3B—C8B—C7B | −3.2 (8) | | |

*Hydrogen-bond geometry (Å, º)*

Cg1 is the centroid of the C3*A*–C8*A* ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C2*B*—H2*D*···O2*B*$^{i}$ | 0.97 | 2.57 | 3.264 (10) | 128 |
| N1*B*—H3···O2*B* | 0.86 (2) | 1.91 (3) | 2.641 (4) | 142 (4) |
| N1*A*—H1···O2*A* | 0.87 (2) | 1.90 (3) | 2.628 (4) | 140 (4) |
| N2*B*—H4···S1*A*$^{ii}$ | 0.84 (2) | 2.68 (2) | 3.469 (3) | 157 (3) |
| N2*A*—H2···S1*B*$^{iii}$ | 0.85 (2) | 2.73 (3) | 3.430 (3) | 140 (3) |
| C12′—H12*C*···*Cg*1$^{iv}$ | 0.90 | 2.49 (2) | 3.42 (1) | 159 |

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