

Crystal structure of 3-[(4-benzylpiperazin-1-yl)methyl]-5-(thiophen-2-yl)-2,3-dihydro-1,3,4-oxadiazole-2-thione

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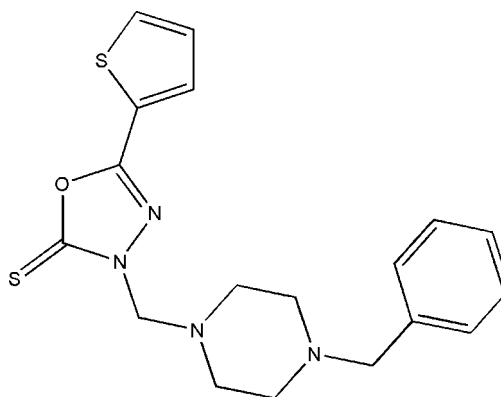
The title 1,3,4-oxadiazole-2-thione derivative, C₁₈H₂₀N₄OS₂, crystallized with two independent molecules (*A* and *B*) in the asymmetric unit. The 2-thienyl rings in both molecules are rotationally disordered over two orientations by approximately 180° about the single C—C bond that connects it to the oxadiazole thione ring; the ratios of site occupancies for the major and minor components were fixed in the structure refinement at 0.8:0.2 and 0.9:0.1 in molecules *A* and *B*, respectively. The 1,3,4-oxadiazole-2-thione ring forms dihedral angles of 7.71 (16), 10.0 (11) and 77.50 (12)° (molecule *A*), and 6.5 (3), 6.0 (9) and 55.30 (12)° (molecule *B*) with the major and minor parts of the disordered thiophene ring and the mean plane of the adjacent piperazine ring, respectively, resulting in approximately V-shaped conformations for the molecules. The piperazine ring in both molecules adopts a chair conformation. The terminal benzene ring is inclined towards the mean plane of the piperazine ring with N—C—C—C torsion angles of −58.2 (3) and −66.2 (3)° in molecules *A* and *B*, respectively. In the crystal, no intermolecular hydrogen bonds are observed. The crystal packing features short S···S contacts [3.4792 (9) Å] and π–π interactions [3.661 (3), 3.664 (11) and 3.5727 (10) Å], producing a three-dimensional network.

Keywords: crystal structure; 1,3,4-oxadiazole; piperazin-1-yl; disorder; π–π interactions; S···S contacts.

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1. Related literature

For the biological activity of 1,3,4-oxadiazole derivatives, see: Al-Deeb *et al.* (2006); El-Emam *et al.* (2004); Kadi *et al.* (2007); Padmavathi *et al.* (2009). For the synthesis of the title compound, see: Al-Omar (2010). For related 1,3,4-oxadiazole structures, see: El-Emam *et al.* (2012, 2013).



2. Experimental

2.1. Crystal data

| | |
|--|--------------------------------------|
| C ₁₈ H ₂₀ N ₄ OS ₂ | <i>V</i> = 3740.4 (3) Å ³ |
| <i>M_r</i> = 372.50 | <i>Z</i> = 8 |
| Monoclinic, <i>P</i> 2 ₁ / <i>c</i> | Mo <i>K</i> α radiation |
| <i>a</i> = 10.6909 (5) Å | <i>μ</i> = 0.30 mm ^{−1} |
| <i>b</i> = 29.3658 (13) Å | <i>T</i> = 273 K |
| <i>c</i> = 15.6179 (6) Å | 0.41 × 0.36 × 0.14 mm |
| <i>β</i> = 130.283 (2)° | |

2.2. Data collection

| | |
|----------------------------------|--|
| Bruker APEXII CCD diffractometer | 11407 independent reflections |
| 88935 measured reflections | 10339 reflections with <i>I</i> > 2σ(<i>I</i>) |
| | <i>R</i> _{int} = 0.034 |

2.3. Refinement

| | |
|---|---|
| <i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)] = 0.059 | 18 restraints |
| <i>wR</i> (<i>F</i> ²) = 0.122 | H-atom parameters constrained |
| <i>S</i> = 1.19 | Δ <i>ρ</i> _{max} = 0.38 e Å ^{−3} |
| 11407 reflections | Δ <i>ρ</i> _{min} = −0.42 e Å ^{−3} |
| 485 parameters | |

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick 2008); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2015); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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§ Thomson Reuters ResearcherID: A-3561-2009.

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Supporting information for this paper is available from the IUCr electronic archives (Reference: SJ5443).

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supporting information

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Crystal structure of 3-[(4-benzylpiperazin-1-yl)methyl]-5-(thiophen-2-yl)-2,3-dihydro-1,3,4-oxadiazole-2-thione

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S1. Chemical context

Considerable attention has been devoted to 1,3,4-oxadiazole derivatives which have long been known for their diverse chemotherapeutic properties as antiviral agents against HIV-1 viruses (El-Emam *et al.*, 2004) and to demonstrate anti-bacterial (Padmavathi *et al.*, 2009) and anti-inflammatory properties (Kadi *et al.*, 2007; Al-Deeb *et al.*, 2006). The title compound was synthesized among a series of 2-thienyl-1,3,4-oxadiazoles and related derivatives as potential anti-microbial agents (Al-Omar, 2010).

S2. Structural commentary

The asymmetric unit of the title compound consists of two crystallographically independent molecules (*A* and *B*) as shown in Fig. 1. The thiophene rings has an approximately 180° rotational disorder (atoms of the minor part are labelled with the suffix *X* and *Y* for molecules *A* and *B*, respectively) about the C2–C3 single bond. The bond lengths and angles are within normal ranges and are comparable with those reported earlier for similar structures (El-Emam *et al.* 2012, 2013). The ratio of the refined site-occupancy factors of the major and minor parts of the disordered thiophene ring is 0.8:0.2 and 0.9 : 0.1 in molecules *A* and *B* respectively. The 1,3,4-oxadiazole-2-thione (O1A/N1A/N2A/C1A/C2A and O1B/N1B/N2B/C1B/C2B) rings form dihedral angles of 7.71 (16), 10.0 (11) and 77.50 (12)° (molecule *A*); and 6.5 (3), 6.0 (9) and 55.30 (12)° (molecule *B*) with the major and minor parts of the disordered thiophene ring and the mean plane of the adjacent piperazine rings (N3A/N4A/C8A–C11A and N3B/N4B/C8B–C11B), resulting in approximately V-shaped conformations for the molecules. The piperazine adopts a chair conformation with puckering parameters: $Q = 0.591$ (2) Å, $\theta = 178.50$ (19)°, and $\varphi = 8(10)$ ° in molecule *A* and $Q = 0.589$ (2) Å, $\theta = 3.10$ (19)°, and $\varphi = 178$ (6)° in molecule *B*. The terminal benzene rings (C13A–C18A and C13B–C18B) in both the molecules are inclined towards the mean plane of the piperazine ring with torsion angles N4A–C12A–C13A–C14A of -58.2 (3)° and N4B–C12B–C13B–C18B of -66.2 (3)°.

S3. Supramolecular features

In the crystal, no significant intermolecular hydrogen bonds are observed. The crystal packing (Fig. 2) is stabilized by a short S··S contact [3.4792 (9) Å] and π – π interactions with Cg1··Cg2ⁱ distance = 3.661 (3) Å, Cg1··Cg3ⁱ distance = 3.664 (11) Å and Cg4··Cg5ⁱ distance = 3.5727 (10) Å (symmetry code: (i) X, Y, Z), producing a three-dimensional structure. Cg1–Cg5 are the centroids of the S2A/C3A/C4A/C5A/C6A, S2B/C3B/C4B/C5B/C6B, C3B/S2Y/C6Y/C5Y/C4Y, O1A/C1A/N2A/N1A/C2A and O1B/C1B/N2B/N1B/C2B rings, respectively.

S4. Synthesis and crystallization

The title compound was prepared by a literature procedure (Al-Omar, 2010) and crystallized from EtOH/CHCl₃ (1:1) to yield colorless crystals. M. P.: 101–103°C.

S5. Refinement details

All H atoms were positioned geometrically (C–H = 0.93 or 0.97 Å) and refined using a riding model with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$. The thienyl ring is disordered over two positions and, in the final refinement cycles, the occupancy ratios were fixed in a ratio 0.8: 0.2 for molecule *A* and 0.9:0.1 for molecule *B*, respectively. Similarity and rigid-bond restraints were applied to the disordered atoms.

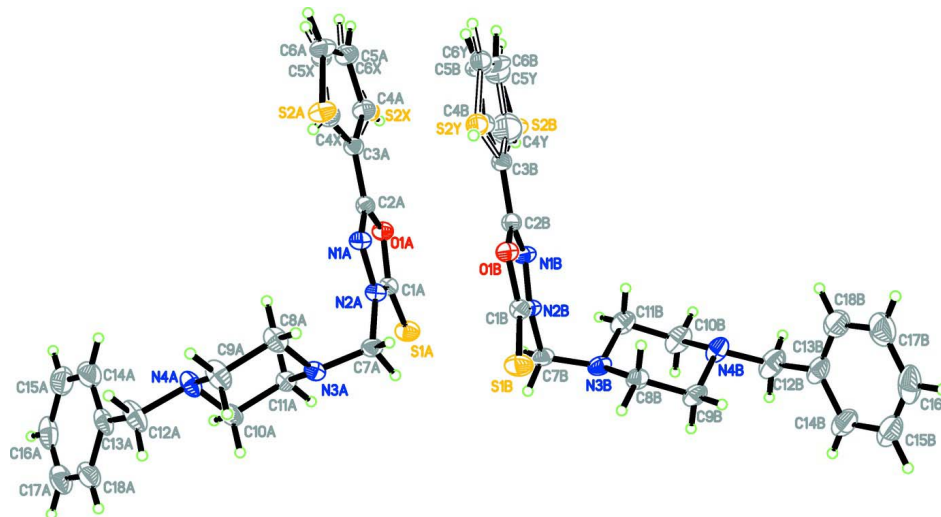
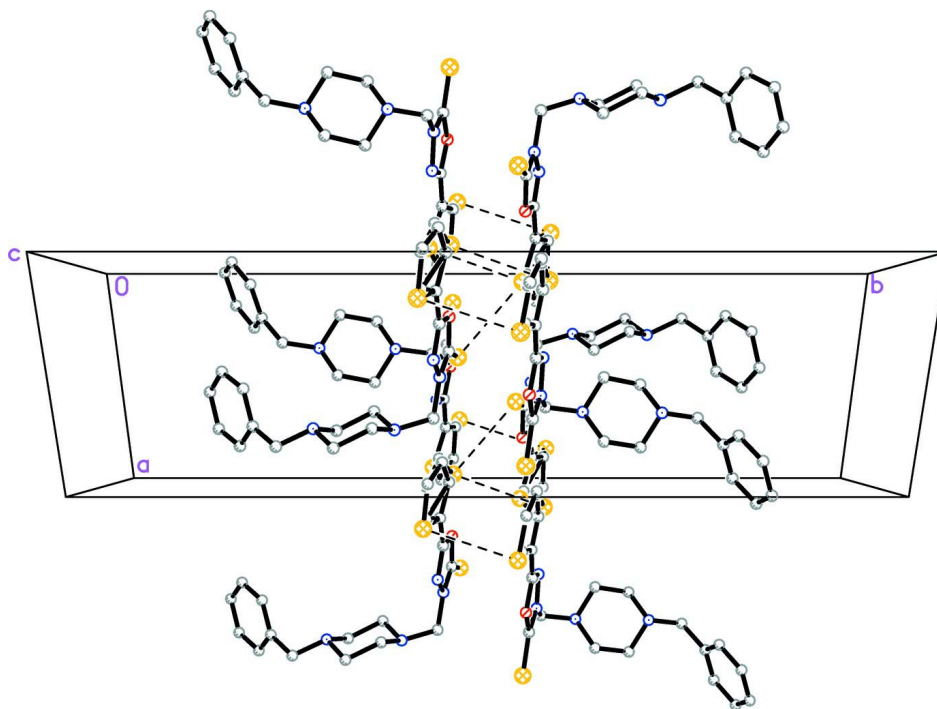


Figure 1

The molecular structure of the title compound with atom labels and 50% probability displacement ellipsoids (atoms of the minor part are labelled with the suffix *X* and *Y* for molecules *A* and *B*, respectively)

**Figure 2**

Crystal packing of the title compound, showing the S...S short contacts and π - π interactions as dashed lines. Only the major components of the thiophene rings are shown. All the H atoms are omitted for clarity.

3-[(4-Benzylpiperazin-1-yl)methyl]-5-(thiophen-2-yl)-2,3-dihydro-1,3,4-oxadiazole-2-thione

Crystal data

$C_{18}H_{20}N_4OS_2$

$M_r = 372.50$

Monoclinic, $P2_1/c$

$a = 10.6909$ (5) Å

$b = 29.3658$ (13) Å

$c = 15.6179$ (6) Å

$\beta = 130.283$ (2)°

$V = 3740.4$ (3) Å³

$Z = 8$

$F(000) = 1568$

$D_x = 1.323$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 9237 reflections

$\theta = 2.4$ – 30.5 °

$\mu = 0.30$ mm⁻¹

$T = 273$ K

Plate, colourless

$0.41 \times 0.36 \times 0.14$ mm

Data collection

Bruker APEXII CCD
diffractometer

φ and ω scans

88935 measured reflections

11407 independent reflections

10339 reflections with $I > 2\sigma(I)$

$R_{int} = 0.034$

$\theta_{max} = 30.6$ °, $\theta_{min} = 2.2$ °

$h = -15$ → 15

$k = -42$ → 41

$l = -22$ → 22

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.059$

$wR(F^2) = 0.122$

$S = 1.19$

11407 reflections

485 parameters

18 restraints

Hydrogen site location: inferred from
neighbouring sites
H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0207P)^2 + 3.9136P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.38 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.42 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ | Occ. (<1) |
|------|--------------|--------------|--------------|----------------------------------|-----------|
| S1B | 0.86597 (6) | 0.54555 (2) | 0.95382 (4) | 0.03328 (11) | |
| O1B | 0.56261 (15) | 0.54910 (4) | 0.88376 (10) | 0.0241 (2) | |
| N1B | 0.40511 (17) | 0.56647 (5) | 0.70234 (13) | 0.0242 (3) | |
| N2B | 0.56914 (17) | 0.56405 (5) | 0.75134 (13) | 0.0240 (3) | |
| N3B | 0.64150 (18) | 0.61694 (6) | 0.66687 (13) | 0.0260 (3) | |
| N4B | 0.64546 (19) | 0.71415 (6) | 0.67316 (13) | 0.0310 (3) | |
| C1B | 0.6665 (2) | 0.55360 (6) | 0.86079 (15) | 0.0241 (3) | |
| C2B | 0.4084 (2) | 0.55740 (6) | 0.78476 (14) | 0.0219 (3) | |
| C3B | 0.2721 (2) | 0.55573 (6) | 0.78285 (15) | 0.0225 (3) | |
| C4B | 0.2698 (4) | 0.54323 (10) | 0.8668 (3) | 0.0270 (6) | 0.8 |
| H4BA | 0.3622 | 0.5338 | 0.9377 | 0.032* | 0.8 |
| C5B | 0.1129 (8) | 0.5463 (4) | 0.8336 (6) | 0.0365 (16) | 0.8 |
| H5BA | 0.0886 | 0.5386 | 0.8793 | 0.044* | 0.8 |
| C6B | 0.0010 (6) | 0.5619 (3) | 0.7273 (5) | 0.0358 (13) | 0.8 |
| H6BA | -0.1088 | 0.5666 | 0.6922 | 0.043* | 0.8 |
| S2B | 0.08174 (8) | 0.57204 (3) | 0.66379 (7) | 0.03174 (14) | 0.8 |
| C4Y | 0.122 (2) | 0.5646 (6) | 0.7033 (14) | 0.055 (5)* | 0.2 |
| H4YA | 0.0848 | 0.5722 | 0.6324 | 0.066* | 0.2 |
| C5Y | 0.015 (3) | 0.5625 (12) | 0.725 (2) | 0.039 (6)* | 0.2 |
| H5YA | -0.0966 | 0.5694 | 0.6747 | 0.046* | 0.2 |
| C6Y | 0.103 (2) | 0.5484 (12) | 0.835 (2) | 0.023 (4)* | 0.2 |
| H6YA | 0.0573 | 0.5449 | 0.8691 | 0.028* | 0.2 |
| S2Y | 0.3049 (4) | 0.53795 (12) | 0.9013 (3) | 0.0243 (7)* | 0.2 |
| C7B | 0.6198 (2) | 0.57087 (7) | 0.68367 (16) | 0.0270 (4) | |
| H7BA | 0.7222 | 0.5548 | 0.7199 | 0.032* | |
| H7BB | 0.5381 | 0.5570 | 0.6107 | 0.032* | |
| C8B | 0.7695 (2) | 0.64187 (6) | 0.77012 (14) | 0.0256 (3) | |
| H8BA | 0.8706 | 0.6245 | 0.8143 | 0.031* | |
| H8BB | 0.7364 | 0.6461 | 0.8146 | 0.031* | |
| C9B | 0.7969 (2) | 0.68769 (7) | 0.74051 (16) | 0.0302 (4) | |
| H9BA | 0.8811 | 0.7042 | 0.8087 | 0.036* | |
| H9BB | 0.8345 | 0.6833 | 0.6988 | 0.036* | |
| C10B | 0.5211 (3) | 0.68905 (8) | 0.56929 (17) | 0.0386 (5) | |
| H10C | 0.5586 | 0.6848 | 0.5275 | 0.046* | |

| | | | | | |
|------|--------------|--------------|--------------|--------------|-----|
| H10D | 0.4201 | 0.7065 | 0.5230 | 0.046* | |
| C11B | 0.4893 (2) | 0.64320 (7) | 0.59601 (16) | 0.0317 (4) | |
| H11C | 0.4467 | 0.6474 | 0.6346 | 0.038* | |
| H11D | 0.4079 | 0.6267 | 0.5269 | 0.038* | |
| C12B | 0.6695 (3) | 0.75944 (8) | 0.64694 (19) | 0.0439 (6) | |
| H12C | 0.5643 | 0.7747 | 0.5963 | 0.053* | |
| H12D | 0.7130 | 0.7563 | 0.6087 | 0.053* | |
| C13B | 0.7846 (2) | 0.78830 (7) | 0.75006 (19) | 0.0365 (5) | |
| C14B | 0.9356 (3) | 0.80127 (8) | 0.7843 (2) | 0.0442 (5) | |
| H14B | 0.9656 | 0.7920 | 0.7428 | 0.053* | |
| C15B | 1.0420 (3) | 0.82762 (8) | 0.8787 (2) | 0.0504 (7) | |
| H15B | 1.1426 | 0.8361 | 0.9002 | 0.061* | |
| C16B | 1.0000 (3) | 0.84134 (8) | 0.9410 (2) | 0.0536 (7) | |
| H16B | 1.0720 | 0.8591 | 1.0048 | 0.064* | |
| C17B | 0.8495 (3) | 0.82871 (8) | 0.9084 (3) | 0.0533 (6) | |
| H17B | 0.8205 | 0.8379 | 0.9505 | 0.064* | |
| C18B | 0.7424 (3) | 0.80236 (8) | 0.8128 (2) | 0.0458 (6) | |
| H18B | 0.6413 | 0.7941 | 0.7909 | 0.055* | |
| S1A | 0.40017 (6) | 0.46380 (2) | 0.54540 (4) | 0.02973 (11) | |
| O1A | 0.22909 (14) | 0.45426 (4) | 0.61460 (10) | 0.0228 (2) | |
| N1A | 0.41622 (17) | 0.43676 (5) | 0.79594 (12) | 0.0224 (3) | |
| N2A | 0.48826 (17) | 0.44323 (5) | 0.74796 (12) | 0.0212 (3) | |
| N3A | 0.71546 (17) | 0.38885 (5) | 0.83070 (12) | 0.0216 (3) | |
| N4A | 0.7102 (2) | 0.29173 (5) | 0.83187 (13) | 0.0288 (3) | |
| C1A | 0.3773 (2) | 0.45354 (6) | 0.63837 (14) | 0.0218 (3) | |
| C2A | 0.2620 (2) | 0.44351 (6) | 0.71288 (14) | 0.0207 (3) | |
| C3A | 0.1288 (2) | 0.44023 (6) | 0.71368 (14) | 0.0218 (3) | |
| C4A | -0.0338 (3) | 0.45153 (8) | 0.6297 (2) | 0.0265 (5) | 0.9 |
| H4AA | -0.0761 | 0.4630 | 0.5601 | 0.032* | 0.9 |
| C5A | -0.1282 (5) | 0.4435 (2) | 0.6622 (4) | 0.0308 (11) | 0.9 |
| H5AA | -0.2400 | 0.4494 | 0.6163 | 0.037* | 0.9 |
| C6A | -0.0374 (5) | 0.4264 (2) | 0.7679 (4) | 0.0303 (9) | 0.9 |
| H6AA | -0.0808 | 0.4187 | 0.8018 | 0.036* | 0.9 |
| S2A | 0.16500 (7) | 0.42031 (2) | 0.83162 (5) | 0.02979 (12) | 0.9 |
| C4X | 0.125 (2) | 0.4241 (7) | 0.7841 (18) | 0.030 (4)* | 0.1 |
| H4XA | 0.2194 | 0.4120 | 0.8506 | 0.036* | 0.1 |
| C5X | -0.025 (4) | 0.424 (2) | 0.762 (3) | 0.022 (6)* | 0.1 |
| H5XA | -0.0411 | 0.4155 | 0.8118 | 0.027* | 0.1 |
| C6X | -0.145 (4) | 0.4397 (16) | 0.654 (3) | 0.010 (5)* | 0.1 |
| H6XA | -0.2563 | 0.4407 | 0.6182 | 0.012* | 0.1 |
| S2X | -0.0673 (7) | 0.45671 (18) | 0.5915 (4) | 0.0191 (11)* | 0.1 |
| C7A | 0.6656 (2) | 0.43542 (6) | 0.81358 (15) | 0.0229 (3) | |
| H7AA | 0.6985 | 0.4506 | 0.7757 | 0.028* | |
| H7AB | 0.7244 | 0.4497 | 0.8864 | 0.028* | |
| C8A | 0.7067 (3) | 0.36412 (7) | 0.90800 (16) | 0.0296 (4) | |
| H8AA | 0.5930 | 0.3599 | 0.8741 | 0.035* | |
| H8AB | 0.7609 | 0.3815 | 0.9766 | 0.035* | |
| C9A | 0.7893 (3) | 0.31819 (7) | 0.93468 (16) | 0.0351 (4) | |

| | | | | |
|------|------------|-------------|--------------|------------|
| H9AA | 0.9042 | 0.3225 | 0.9717 | 0.042* |
| H9AB | 0.7828 | 0.3016 | 0.9854 | 0.042* |
| C10A | 0.7223 (2) | 0.31688 (6) | 0.75678 (15) | 0.0267 (4) |
| H10A | 0.6714 | 0.2994 | 0.6887 | 0.032* |
| H10B | 0.8368 | 0.3213 | 0.7929 | 0.032* |
| C11A | 0.6385 (2) | 0.36268 (6) | 0.72752 (14) | 0.0218 (3) |
| H11A | 0.6480 | 0.3792 | 0.6782 | 0.026* |
| H11B | 0.5230 | 0.3584 | 0.6887 | 0.026* |
| C12A | 0.7871 (3) | 0.24680 (7) | 0.85974 (18) | 0.0402 (5) |
| H12A | 0.7855 | 0.2325 | 0.9150 | 0.048* |
| H12B | 0.9008 | 0.2506 | 0.8933 | 0.048* |
| C13A | 0.7034 (3) | 0.21574 (6) | 0.75928 (17) | 0.0330 (4) |
| C14A | 0.5388 (3) | 0.20464 (8) | 0.6944 (2) | 0.0407 (5) |
| H14A | 0.4774 | 0.2169 | 0.7117 | 0.049* |
| C15A | 0.4650 (3) | 0.17530 (8) | 0.6036 (2) | 0.0450 (5) |
| H15A | 0.3545 | 0.1681 | 0.5605 | 0.054* |
| C16A | 0.5548 (3) | 0.15663 (7) | 0.5769 (2) | 0.0433 (5) |
| H16A | 0.5049 | 0.1372 | 0.5157 | 0.052* |
| C17A | 0.7186 (3) | 0.16709 (7) | 0.6416 (2) | 0.0433 (5) |
| H17A | 0.7800 | 0.1543 | 0.6248 | 0.052* |
| C18A | 0.7922 (3) | 0.19659 (7) | 0.7316 (2) | 0.0382 (5) |
| H18A | 0.9027 | 0.2037 | 0.7742 | 0.046* |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|------|-------------|-------------|-------------|--------------|--------------|--------------|
| S1B | 0.0208 (2) | 0.0416 (3) | 0.0332 (2) | 0.00472 (18) | 0.01552 (19) | 0.0035 (2) |
| O1B | 0.0221 (6) | 0.0267 (6) | 0.0252 (6) | -0.0003 (5) | 0.0160 (5) | -0.0005 (5) |
| N1B | 0.0194 (6) | 0.0317 (8) | 0.0249 (7) | -0.0051 (6) | 0.0159 (6) | -0.0065 (6) |
| N2B | 0.0185 (6) | 0.0310 (8) | 0.0250 (7) | -0.0034 (5) | 0.0152 (6) | -0.0047 (6) |
| N3B | 0.0204 (7) | 0.0353 (8) | 0.0221 (7) | -0.0060 (6) | 0.0137 (6) | -0.0054 (6) |
| N4B | 0.0224 (7) | 0.0316 (8) | 0.0254 (8) | -0.0034 (6) | 0.0094 (6) | 0.0073 (6) |
| C1B | 0.0237 (8) | 0.0220 (8) | 0.0295 (8) | -0.0013 (6) | 0.0186 (7) | -0.0034 (6) |
| C2B | 0.0206 (7) | 0.0219 (8) | 0.0246 (8) | -0.0025 (6) | 0.0153 (7) | -0.0045 (6) |
| C3B | 0.0225 (7) | 0.0228 (8) | 0.0261 (8) | -0.0037 (6) | 0.0174 (7) | -0.0054 (6) |
| C4B | 0.0241 (13) | 0.0294 (13) | 0.0281 (15) | -0.0001 (10) | 0.0171 (13) | -0.0019 (12) |
| C5B | 0.041 (2) | 0.042 (3) | 0.046 (2) | -0.0133 (15) | 0.0372 (19) | -0.0147 (13) |
| C6B | 0.0233 (15) | 0.056 (2) | 0.0382 (18) | -0.0136 (13) | 0.0243 (15) | -0.0155 (13) |
| S2B | 0.0208 (3) | 0.0468 (4) | 0.0288 (3) | -0.0045 (3) | 0.0166 (3) | -0.0058 (3) |
| C7B | 0.0259 (8) | 0.0342 (9) | 0.0297 (9) | -0.0057 (7) | 0.0219 (7) | -0.0085 (7) |
| C8B | 0.0182 (7) | 0.0303 (9) | 0.0216 (8) | -0.0015 (6) | 0.0099 (7) | -0.0016 (7) |
| C9B | 0.0192 (8) | 0.0359 (10) | 0.0273 (9) | -0.0051 (7) | 0.0113 (7) | 0.0011 (7) |
| C10B | 0.0272 (9) | 0.0465 (12) | 0.0224 (9) | -0.0055 (8) | 0.0072 (8) | 0.0069 (8) |
| C11B | 0.0198 (8) | 0.0413 (11) | 0.0220 (8) | -0.0054 (7) | 0.0081 (7) | -0.0003 (7) |
| C12B | 0.0359 (11) | 0.0420 (12) | 0.0372 (11) | -0.0041 (9) | 0.0163 (10) | 0.0159 (9) |
| C13B | 0.0266 (9) | 0.0269 (9) | 0.0408 (11) | 0.0001 (7) | 0.0150 (9) | 0.0139 (8) |
| C14B | 0.0326 (10) | 0.0374 (11) | 0.0535 (14) | -0.0034 (9) | 0.0238 (10) | 0.0112 (10) |
| C15B | 0.0289 (10) | 0.0337 (11) | 0.0622 (16) | -0.0023 (9) | 0.0175 (11) | 0.0104 (11) |

| | | | | | | |
|------|-------------|-------------|-------------|--------------|--------------|--------------|
| C16B | 0.0430 (13) | 0.0246 (10) | 0.0505 (14) | 0.0019 (9) | 0.0110 (11) | 0.0058 (10) |
| C17B | 0.0570 (15) | 0.0327 (12) | 0.0638 (17) | 0.0086 (11) | 0.0363 (14) | 0.0064 (11) |
| C18B | 0.0333 (11) | 0.0344 (11) | 0.0604 (15) | 0.0036 (9) | 0.0261 (11) | 0.0099 (10) |
| S1A | 0.0307 (2) | 0.0384 (3) | 0.0258 (2) | 0.00467 (19) | 0.02082 (19) | 0.00510 (18) |
| O1A | 0.0198 (5) | 0.0271 (6) | 0.0211 (6) | 0.0010 (5) | 0.0130 (5) | 0.0004 (5) |
| N1A | 0.0204 (6) | 0.0269 (7) | 0.0221 (7) | -0.0001 (5) | 0.0147 (6) | -0.0013 (5) |
| N2A | 0.0195 (6) | 0.0243 (7) | 0.0216 (6) | 0.0011 (5) | 0.0141 (6) | -0.0001 (5) |
| N3A | 0.0192 (6) | 0.0242 (7) | 0.0200 (6) | 0.0013 (5) | 0.0120 (6) | -0.0014 (5) |
| N4A | 0.0396 (9) | 0.0247 (7) | 0.0245 (7) | 0.0114 (6) | 0.0218 (7) | 0.0063 (6) |
| C1A | 0.0209 (7) | 0.0202 (7) | 0.0245 (8) | 0.0012 (6) | 0.0148 (7) | -0.0002 (6) |
| C2A | 0.0217 (7) | 0.0200 (7) | 0.0217 (7) | -0.0002 (6) | 0.0146 (6) | -0.0020 (6) |
| C3A | 0.0194 (7) | 0.0225 (8) | 0.0230 (8) | -0.0011 (6) | 0.0135 (6) | -0.0024 (6) |
| C4A | 0.0231 (10) | 0.0308 (11) | 0.0251 (12) | -0.0005 (8) | 0.0154 (10) | -0.0001 (10) |
| C5A | 0.0218 (14) | 0.033 (2) | 0.0358 (17) | -0.0034 (13) | 0.0179 (13) | -0.0032 (13) |
| C6A | 0.0215 (12) | 0.0390 (17) | 0.0345 (14) | -0.0028 (10) | 0.0200 (11) | -0.0025 (11) |
| S2A | 0.0218 (2) | 0.0423 (3) | 0.0259 (3) | -0.0006 (2) | 0.0158 (2) | 0.0029 (2) |
| C7A | 0.0170 (7) | 0.0260 (8) | 0.0239 (8) | -0.0023 (6) | 0.0123 (6) | -0.0037 (6) |
| C8A | 0.0387 (10) | 0.0305 (9) | 0.0233 (8) | 0.0077 (8) | 0.0218 (8) | 0.0032 (7) |
| C9A | 0.0461 (12) | 0.0333 (10) | 0.0218 (8) | 0.0142 (9) | 0.0201 (9) | 0.0061 (7) |
| C10A | 0.0304 (9) | 0.0285 (9) | 0.0244 (8) | 0.0067 (7) | 0.0191 (7) | 0.0019 (7) |
| C11A | 0.0228 (7) | 0.0235 (8) | 0.0185 (7) | 0.0012 (6) | 0.0130 (6) | 0.0006 (6) |
| C12A | 0.0545 (13) | 0.0310 (10) | 0.0327 (10) | 0.0205 (9) | 0.0272 (10) | 0.0101 (8) |
| C13A | 0.0525 (12) | 0.0221 (8) | 0.0351 (10) | 0.0144 (8) | 0.0331 (10) | 0.0109 (7) |
| C14A | 0.0559 (14) | 0.0341 (11) | 0.0505 (13) | 0.0101 (10) | 0.0427 (12) | 0.0072 (9) |
| C15A | 0.0579 (15) | 0.0338 (11) | 0.0504 (14) | 0.0004 (10) | 0.0382 (13) | 0.0051 (10) |
| C16A | 0.0722 (17) | 0.0240 (9) | 0.0413 (12) | 0.0055 (10) | 0.0402 (12) | 0.0065 (8) |
| C17A | 0.0719 (16) | 0.0300 (10) | 0.0500 (13) | 0.0129 (10) | 0.0493 (13) | 0.0064 (9) |
| C18A | 0.0518 (13) | 0.0305 (10) | 0.0456 (12) | 0.0117 (9) | 0.0374 (11) | 0.0063 (9) |

Geometric parameters (Å, °)

| | | | |
|----------|-------------|----------|-------------|
| S1B—C1B | 1.6452 (18) | S1A—C1A | 1.6484 (18) |
| O1B—C2B | 1.368 (2) | O1A—C2A | 1.372 (2) |
| O1B—C1B | 1.377 (2) | O1A—C1A | 1.374 (2) |
| N1B—C2B | 1.293 (2) | N1A—C2A | 1.294 (2) |
| N1B—N2B | 1.3894 (19) | N1A—N2A | 1.3917 (19) |
| N2B—C1B | 1.341 (2) | N2A—C1A | 1.343 (2) |
| N2B—C7B | 1.481 (2) | N2A—C7A | 1.478 (2) |
| N3B—C7B | 1.425 (2) | N3A—C7A | 1.429 (2) |
| N3B—C11B | 1.463 (2) | N3A—C8A | 1.463 (2) |
| N3B—C8B | 1.468 (2) | N3A—C11A | 1.466 (2) |
| N4B—C9B | 1.459 (2) | N4A—C10A | 1.461 (2) |
| N4B—C12B | 1.463 (3) | N4A—C9A | 1.463 (2) |
| N4B—C10B | 1.467 (3) | N4A—C12A | 1.464 (2) |
| C2B—C3B | 1.439 (2) | C2A—C3A | 1.436 (2) |
| C3B—C4Y | 1.267 (17) | C3A—C4X | 1.22 (2) |
| C3B—C4B | 1.377 (4) | C3A—C4A | 1.380 (3) |
| C3B—S2B | 1.7132 (19) | C3A—S2A | 1.7213 (18) |

| | | | |
|--------------|-------------|--------------|-------------|
| C3B—S2Y | 1.726 (4) | C3A—S2X | 1.759 (6) |
| C4B—C5B | 1.403 (6) | C4A—C5A | 1.411 (4) |
| C4B—H4BA | 0.9300 | C4A—H4AA | 0.9300 |
| C5B—C6B | 1.353 (5) | C5A—C6A | 1.360 (4) |
| C5B—H5BA | 0.9300 | C5A—H5AA | 0.9300 |
| C6B—S2B | 1.710 (5) | C6A—S2A | 1.709 (4) |
| C6B—H6BA | 0.9300 | C6A—H6AA | 0.9300 |
| C4Y—C5Y | 1.395 (18) | C4X—C5X | 1.413 (19) |
| C4Y—H4YA | 0.9300 | C4X—H4XA | 0.9300 |
| C5Y—C6Y | 1.384 (15) | C5X—C6X | 1.383 (17) |
| C5Y—H5YA | 0.9300 | C5X—H5XA | 0.9300 |
| C6Y—S2Y | 1.716 (18) | C6X—S2X | 1.712 (19) |
| C6Y—H6YA | 0.9300 | C6X—H6XA | 0.9300 |
| C7B—H7BA | 0.9700 | C7A—H7AA | 0.9700 |
| C7B—H7BB | 0.9700 | C7A—H7AB | 0.9700 |
| C8B—C9B | 1.512 (3) | C8A—C9A | 1.515 (3) |
| C8B—H8BA | 0.9700 | C8A—H8AA | 0.9700 |
| C8B—H8BB | 0.9700 | C8A—H8AB | 0.9700 |
| C9B—H9BA | 0.9700 | C9A—H9AA | 0.9700 |
| C9B—H9BB | 0.9700 | C9A—H9AB | 0.9700 |
| C10B—C11B | 1.512 (3) | C10A—C11A | 1.513 (2) |
| C10B—H10C | 0.9700 | C10A—H10A | 0.9700 |
| C10B—H10D | 0.9700 | C10A—H10B | 0.9700 |
| C11B—H11C | 0.9700 | C11A—H11A | 0.9700 |
| C11B—H11D | 0.9700 | C11A—H11B | 0.9700 |
| C12B—C13B | 1.504 (3) | C12A—C13A | 1.510 (3) |
| C12B—H12C | 0.9700 | C12A—H12A | 0.9700 |
| C12B—H12D | 0.9700 | C12A—H12B | 0.9700 |
| C13B—C18B | 1.381 (4) | C13A—C14A | 1.387 (3) |
| C13B—C14B | 1.386 (3) | C13A—C18A | 1.391 (3) |
| C14B—C15B | 1.378 (4) | C14A—C15A | 1.388 (3) |
| C14B—H14B | 0.9300 | C14A—H14A | 0.9300 |
| C15B—C16B | 1.369 (4) | C15A—C16A | 1.384 (3) |
| C15B—H15B | 0.9300 | C15A—H15A | 0.9300 |
| C16B—C17B | 1.389 (4) | C16A—C17A | 1.375 (4) |
| C16B—H16B | 0.9300 | C16A—H16A | 0.9300 |
| C17B—C18B | 1.388 (4) | C17A—C18A | 1.384 (3) |
| C17B—H17B | 0.9300 | C17A—H17A | 0.9300 |
| C18B—H18B | 0.9300 | C18A—H18A | 0.9300 |
| | | | |
| C2B—O1B—C1B | 105.92 (13) | C2A—O1A—C1A | 106.11 (13) |
| C2B—N1B—N2B | 103.24 (14) | C2A—N1A—N2A | 103.26 (13) |
| C1B—N2B—N1B | 112.16 (14) | C1A—N2A—N1A | 112.15 (13) |
| C1B—N2B—C7B | 126.86 (15) | C1A—N2A—C7A | 126.78 (14) |
| N1B—N2B—C7B | 120.94 (14) | N1A—N2A—C7A | 120.91 (14) |
| C7B—N3B—C11B | 113.95 (15) | C7A—N3A—C8A | 114.47 (14) |
| C7B—N3B—C8B | 114.72 (15) | C7A—N3A—C11A | 114.82 (14) |
| C11B—N3B—C8B | 111.03 (15) | C8A—N3A—C11A | 110.91 (14) |

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|---------------|-------------|---------------|-------------|
| C9B—N4B—C12B | 111.82 (16) | C10A—N4A—C9A | 108.92 (16) |
| C9B—N4B—C10B | 108.63 (17) | C10A—N4A—C12A | 111.72 (16) |
| C12B—N4B—C10B | 110.18 (16) | C9A—N4A—C12A | 109.72 (15) |
| N2B—C1B—O1B | 105.16 (14) | N2A—C1A—O1A | 105.17 (14) |
| N2B—C1B—S1B | 130.80 (14) | N2A—C1A—S1A | 130.72 (13) |
| O1B—C1B—S1B | 124.01 (14) | O1A—C1A—S1A | 124.11 (13) |
| N1B—C2B—O1B | 113.52 (14) | N1A—C2A—O1A | 113.30 (14) |
| N1B—C2B—C3B | 127.69 (16) | N1A—C2A—C3A | 127.53 (16) |
| O1B—C2B—C3B | 118.79 (15) | O1A—C2A—C3A | 119.16 (15) |
| C4Y—C3B—C2B | 129.5 (7) | C4X—C3A—C2A | 130.0 (9) |
| C4B—C3B—C2B | 129.1 (2) | C4A—C3A—C2A | 128.50 (18) |
| C4B—C3B—S2B | 111.59 (17) | C4A—C3A—S2A | 111.88 (15) |
| C2B—C3B—S2B | 119.30 (13) | C2A—C3A—S2A | 119.61 (13) |
| C4Y—C3B—S2Y | 111.4 (7) | C4X—C3A—S2X | 112.0 (10) |
| C2B—C3B—S2Y | 119.13 (17) | C2A—C3A—S2X | 117.7 (2) |
| C3B—C4B—C5B | 112.6 (4) | C3A—C4A—C5A | 111.8 (3) |
| C3B—C4B—H4BA | 123.7 | C3A—C4A—H4AA | 124.1 |
| C5B—C4B—H4BA | 123.7 | C5A—C4A—H4AA | 124.1 |
| C6B—C5B—C4B | 111.8 (5) | C6A—C5A—C4A | 112.5 (4) |
| C6B—C5B—H5BA | 124.1 | C6A—C5A—H5AA | 123.7 |
| C4B—C5B—H5BA | 124.1 | C4A—C5A—H5AA | 123.7 |
| C5B—C6B—S2B | 113.2 (4) | C5A—C6A—S2A | 112.7 (3) |
| C5B—C6B—H6BA | 123.4 | C5A—C6A—H6AA | 123.6 |
| S2B—C6B—H6BA | 123.4 | S2A—C6A—H6AA | 123.6 |
| C6B—S2B—C3B | 90.74 (19) | C6A—S2A—C3A | 90.99 (14) |
| C3B—C4Y—C5Y | 118.1 (15) | C3A—C4X—C5X | 118.3 (18) |
| C3B—C4Y—H4YA | 120.9 | C3A—C4X—H4XA | 120.8 |
| C5Y—C4Y—H4YA | 120.9 | C5X—C4X—H4XA | 120.8 |
| C6Y—C5Y—C4Y | 108.0 (19) | C6X—C5X—C4X | 108 (2) |
| C6Y—C5Y—H5YA | 126.0 | C6X—C5X—H5XA | 126.1 |
| C4Y—C5Y—H5YA | 126.0 | C4X—C5X—H5XA | 126.1 |
| C5Y—C6Y—S2Y | 112.5 (17) | C5X—C6X—S2X | 112.6 (19) |
| C5Y—C6Y—H6YA | 123.7 | C5X—C6X—H6XA | 123.7 |
| S2Y—C6Y—H6YA | 123.7 | S2X—C6X—H6XA | 123.7 |
| C6Y—S2Y—C3B | 89.7 (8) | C6X—S2X—C3A | 88.9 (10) |
| N3B—C7B—N2B | 115.96 (15) | N3A—C7A—N2A | 115.75 (14) |
| N3B—C7B—H7BA | 108.3 | N3A—C7A—H7AA | 108.3 |
| N2B—C7B—H7BA | 108.3 | N2A—C7A—H7AA | 108.3 |
| N3B—C7B—H7BB | 108.3 | N3A—C7A—H7AB | 108.3 |
| N2B—C7B—H7BB | 108.3 | N2A—C7A—H7AB | 108.3 |
| H7BA—C7B—H7BB | 107.4 | H7AA—C7A—H7AB | 107.4 |
| N3B—C8B—C9B | 109.59 (15) | N3A—C8A—C9A | 109.39 (15) |
| N3B—C8B—H8BA | 109.8 | N3A—C8A—H8AA | 109.8 |
| C9B—C8B—H8BA | 109.8 | C9A—C8A—H8AA | 109.8 |
| N3B—C8B—H8BB | 109.8 | N3A—C8A—H8AB | 109.8 |
| C9B—C8B—H8BB | 109.8 | C9A—C8A—H8AB | 109.8 |
| H8BA—C8B—H8BB | 108.2 | H8AA—C8A—H8AB | 108.2 |
| N4B—C9B—C8B | 110.47 (15) | N4A—C9A—C8A | 110.51 (15) |

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|-----------------|--------------|-----------------|--------------|
| N4B—C9B—H9BA | 109.6 | N4A—C9A—H9AA | 109.5 |
| C8B—C9B—H9BA | 109.6 | C8A—C9A—H9AA | 109.5 |
| N4B—C9B—H9BB | 109.6 | N4A—C9A—H9AB | 109.5 |
| C8B—C9B—H9BB | 109.6 | C8A—C9A—H9AB | 109.5 |
| H9BA—C9B—H9BB | 108.1 | H9AA—C9A—H9AB | 108.1 |
| N4B—C10B—C11B | 110.30 (16) | N4A—C10A—C11A | 110.44 (14) |
| N4B—C10B—H10C | 109.6 | N4A—C10A—H10A | 109.6 |
| C11B—C10B—H10C | 109.6 | C11A—C10A—H10A | 109.6 |
| N4B—C10B—H10D | 109.6 | N4A—C10A—H10B | 109.6 |
| C11B—C10B—H10D | 109.6 | C11A—C10A—H10B | 109.6 |
| H10C—C10B—H10D | 108.1 | H10A—C10A—H10B | 108.1 |
| N3B—C11B—C10B | 109.84 (16) | N3A—C11A—C10A | 109.39 (14) |
| N3B—C11B—H11C | 109.7 | N3A—C11A—H11A | 109.8 |
| C10B—C11B—H11C | 109.7 | C10A—C11A—H11A | 109.8 |
| N3B—C11B—H11D | 109.7 | N3A—C11A—H11B | 109.8 |
| C10B—C11B—H11D | 109.7 | C10A—C11A—H11B | 109.8 |
| H11C—C11B—H11D | 108.2 | H11A—C11A—H11B | 108.2 |
| N4B—C12B—C13B | 112.51 (17) | N4A—C12A—C13A | 113.20 (17) |
| N4B—C12B—H12C | 109.1 | N4A—C12A—H12A | 108.9 |
| C13B—C12B—H12C | 109.1 | C13A—C12A—H12A | 108.9 |
| N4B—C12B—H12D | 109.1 | N4A—C12A—H12B | 108.9 |
| C13B—C12B—H12D | 109.1 | C13A—C12A—H12B | 108.9 |
| H12C—C12B—H12D | 107.8 | H12A—C12A—H12B | 107.8 |
| C18B—C13B—C14B | 118.5 (2) | C14A—C13A—C18A | 118.5 (2) |
| C18B—C13B—C12B | 120.8 (2) | C14A—C13A—C12A | 121.40 (19) |
| C14B—C13B—C12B | 120.7 (2) | C18A—C13A—C12A | 120.1 (2) |
| C15B—C14B—C13B | 121.2 (3) | C13A—C14A—C15A | 120.5 (2) |
| C15B—C14B—H14B | 119.4 | C13A—C14A—H14A | 119.8 |
| C13B—C14B—H14B | 119.4 | C15A—C14A—H14A | 119.8 |
| C16B—C15B—C14B | 120.1 (2) | C16A—C15A—C14A | 120.4 (3) |
| C16B—C15B—H15B | 119.9 | C16A—C15A—H15A | 119.8 |
| C14B—C15B—H15B | 119.9 | C14A—C15A—H15A | 119.8 |
| C15B—C16B—C17B | 119.7 (3) | C17A—C16A—C15A | 119.4 (2) |
| C15B—C16B—H16B | 120.1 | C17A—C16A—H16A | 120.3 |
| C17B—C16B—H16B | 120.1 | C15A—C16A—H16A | 120.3 |
| C18B—C17B—C16B | 119.8 (3) | C16A—C17A—C18A | 120.3 (2) |
| C18B—C17B—H17B | 120.1 | C16A—C17A—H17A | 119.8 |
| C16B—C17B—H17B | 120.1 | C18A—C17A—H17A | 119.8 |
| C13B—C18B—C17B | 120.6 (2) | C17A—C18A—C13A | 120.9 (2) |
| C13B—C18B—H18B | 119.7 | C17A—C18A—H18A | 119.5 |
| C17B—C18B—H18B | 119.7 | C13A—C18A—H18A | 119.5 |
| | | | |
| C2B—N1B—N2B—C1B | 0.15 (19) | C2A—N1A—N2A—C1A | -0.09 (19) |
| C2B—N1B—N2B—C7B | 177.93 (16) | C2A—N1A—N2A—C7A | -175.66 (15) |
| N1B—N2B—C1B—O1B | -0.04 (19) | N1A—N2A—C1A—O1A | 0.61 (18) |
| C7B—N2B—C1B—O1B | -177.65 (16) | C7A—N2A—C1A—O1A | 175.86 (15) |
| N1B—N2B—C1B—S1B | 178.23 (14) | N1A—N2A—C1A—S1A | -179.50 (13) |
| C7B—N2B—C1B—S1B | 0.6 (3) | C7A—N2A—C1A—S1A | -4.2 (3) |

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| C2B—O1B—C1B—N2B | -0.08 (18) | C2A—O1A—C1A—N2A | -0.86 (17) |
| C2B—O1B—C1B—S1B | -178.50 (13) | C2A—O1A—C1A—S1A | 179.24 (13) |
| N2B—N1B—C2B—O1B | -0.21 (19) | N2A—N1A—C2A—O1A | -0.50 (18) |
| N2B—N1B—C2B—C3B | 179.12 (17) | N2A—N1A—C2A—C3A | 178.47 (16) |
| C1B—O1B—C2B—N1B | 0.19 (19) | C1A—O1A—C2A—N1A | 0.88 (19) |
| C1B—O1B—C2B—C3B | -179.20 (15) | C1A—O1A—C2A—C3A | -178.17 (15) |
| N1B—C2B—C3B—C4Y | -3.6 (11) | N1A—C2A—C3A—C4X | -12.6 (14) |
| O1B—C2B—C3B—C4Y | 175.7 (11) | O1A—C2A—C3A—C4X | 166.3 (14) |
| N1B—C2B—C3B—C4B | 175.1 (2) | N1A—C2A—C3A—C4A | 173.0 (2) |
| O1B—C2B—C3B—C4B | -5.6 (3) | O1A—C2A—C3A—C4A | -8.1 (3) |
| N1B—C2B—C3B—S2B | -6.3 (3) | N1A—C2A—C3A—S2A | -6.5 (3) |
| O1B—C2B—C3B—S2B | 172.95 (12) | O1A—C2A—C3A—S2A | 172.39 (12) |
| N1B—C2B—C3B—S2Y | 174.4 (2) | N1A—C2A—C3A—S2X | 173.9 (2) |
| O1B—C2B—C3B—S2Y | -6.3 (3) | O1A—C2A—C3A—S2X | -7.2 (3) |
| C4Y—C3B—C4B—C5B | -1.6 (10) | C4X—C3A—C4A—C5A | 4.5 (11) |
| C2B—C3B—C4B—C5B | 179.5 (5) | C2A—C3A—C4A—C5A | -179.9 (3) |
| S2B—C3B—C4B—C5B | 0.9 (5) | S2A—C3A—C4A—C5A | -0.4 (4) |
| S2Y—C3B—C4B—C5B | -176.9 (15) | S2X—C3A—C4A—C5A | 175.8 (14) |
| C3B—C4B—C5B—C6B | -1.4 (10) | C3A—C4A—C5A—C6A | -0.4 (6) |
| C4B—C5B—C6B—S2B | 1.3 (10) | C4A—C5A—C6A—S2A | 1.0 (7) |
| C5B—C6B—S2B—C3B | -0.7 (7) | C5A—C6A—S2A—C3A | -1.0 (5) |
| C4Y—C3B—S2B—C6B | 13 (5) | C4X—C3A—S2A—C6A | -24 (5) |
| C4B—C3B—S2B—C6B | -0.1 (3) | C4A—C3A—S2A—C6A | 0.8 (3) |
| C2B—C3B—S2B—C6B | -178.9 (3) | C2A—C3A—S2A—C6A | -179.6 (3) |
| S2Y—C3B—S2B—C6B | 0.3 (3) | S2X—C3A—S2A—C6A | -0.1 (3) |
| C4B—C3B—C4Y—C5Y | 4 (2) | C4A—C3A—C4X—C5X | -3 (3) |
| C2B—C3B—C4Y—C5Y | -176.7 (18) | C2A—C3A—C4X—C5X | -178 (3) |
| S2B—C3B—C4Y—C5Y | -163 (6) | S2A—C3A—C4X—C5X | 154 (7) |
| S2Y—C3B—C4Y—C5Y | 5 (2) | S2X—C3A—C4X—C5X | -5 (4) |
| C3B—C4Y—C5Y—C6Y | -3 (4) | C3A—C4X—C5X—C6X | 6 (6) |
| C4Y—C5Y—C6Y—S2Y | -1 (4) | C4X—C5X—C6X—S2X | -5 (6) |
| C5Y—C6Y—S2Y—C3B | 3 (3) | C5X—C6X—S2X—C3A | 2 (4) |
| C4Y—C3B—S2Y—C6Y | -4.6 (16) | C4X—C3A—S2X—C6X | 1 (2) |
| C4B—C3B—S2Y—C6Y | 0.3 (17) | C4A—C3A—S2X—C6X | -8 (2) |
| C2B—C3B—S2Y—C6Y | 177.1 (13) | C2A—C3A—S2X—C6X | 175.9 (17) |
| S2B—C3B—S2Y—C6Y | -2.1 (13) | S2A—C3A—S2X—C6X | -3.6 (17) |
| C11B—N3B—C7B—N2B | -68.0 (2) | C8A—N3A—C7A—N2A | -70.88 (19) |
| C8B—N3B—C7B—N2B | 61.6 (2) | C11A—N3A—C7A—N2A | 59.11 (19) |
| C1B—N2B—C7B—N3B | -98.4 (2) | C1A—N2A—C7A—N3A | -98.7 (2) |
| N1B—N2B—C7B—N3B | 84.2 (2) | N1A—N2A—C7A—N3A | 76.1 (2) |
| C7B—N3B—C8B—C9B | 172.08 (15) | C7A—N3A—C8A—C9A | -170.33 (16) |
| C11B—N3B—C8B—C9B | -56.94 (19) | C11A—N3A—C8A—C9A | 57.8 (2) |
| C12B—N4B—C9B—C8B | 177.67 (18) | C10A—N4A—C9A—C8A | 59.8 (2) |
| C10B—N4B—C9B—C8B | -60.5 (2) | C12A—N4A—C9A—C8A | -177.65 (19) |
| N3B—C8B—C9B—N4B | 59.0 (2) | N3A—C8A—C9A—N4A | -58.7 (2) |
| C9B—N4B—C10B—C11B | 60.3 (2) | C9A—N4A—C10A—C11A | -59.9 (2) |
| C12B—N4B—C10B—C11B | -176.93 (19) | C12A—N4A—C10A—C11A | 178.73 (17) |
| C7B—N3B—C11B—C10B | -171.68 (16) | C7A—N3A—C11A—C10A | 170.34 (14) |

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| C8B—N3B—C11B—C10B | 56.9 (2) | C8A—N3A—C11A—C10A | -57.95 (18) |
| N4B—C10B—C11B—N3B | -58.7 (2) | N4A—C10A—C11A—N3A | 59.00 (19) |
| C9B—N4B—C12B—C13B | -64.3 (3) | C10A—N4A—C12A—C13A | -64.0 (2) |
| C10B—N4B—C12B—C13B | 174.8 (2) | C9A—N4A—C12A—C13A | 175.08 (19) |
| N4B—C12B—C13B—C18B | -66.2 (3) | N4A—C12A—C13A—C14A | -58.2 (3) |
| N4B—C12B—C13B—C14B | 113.6 (2) | N4A—C12A—C13A—C18A | 123.5 (2) |
| C18B—C13B—C14B—C15B | 0.0 (3) | C18A—C13A—C14A—C15A | -0.4 (3) |
| C12B—C13B—C14B—C15B | -179.9 (2) | C12A—C13A—C14A—C15A | -178.7 (2) |
| C13B—C14B—C15B—C16B | 0.3 (4) | C13A—C14A—C15A—C16A | 0.2 (3) |
| C14B—C15B—C16B—C17B | -0.2 (4) | C14A—C15A—C16A—C17A | 0.5 (3) |
| C15B—C16B—C17B—C18B | -0.2 (4) | C15A—C16A—C17A—C18A | -1.0 (3) |
| C14B—C13B—C18B—C17B | -0.3 (3) | C16A—C17A—C18A—C13A | 0.8 (3) |
| C12B—C13B—C18B—C17B | 179.5 (2) | C14A—C13A—C18A—C17A | -0.1 (3) |
| C16B—C17B—C18B—C13B | 0.4 (4) | C12A—C13A—C18A—C17A | 178.27 (19) |
