Dimethyl DL-2,3-dibenzyl-2,3-diisothiocyanatosuccinate

Justyna Kalinowska-Tłusćik,* Dariusz Ciez and Sandrine Peyrat

The title compound, C_{22}H_{30}N_{2}O_{5}S_{2}, has approximate molecular twofold symmetry. In the crystal, the presence of C—H···H interactions leads to the formation of zigzag chains along [001].

Related literature

For the synthesis and spectroscopic characterization of the title compound, see: Ciez’ (2007). For the synthesis, spectroscopic characterization and crystal structure determination of similar compounds, see: Ciez et al. (2008). For diisothiocyanates, see: Morel & Marchand (2001). For C—H···π and C—H···O interactions, see: Malone et al. (1997); Arunan et al. (2011a,b).

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan
(DENZO-SMN; Otwinowski & Minor, 1997)
T_{	ext{min}} = 0.926, T_{	ext{max}} = 0.952
9175 measured reflections
4868 independent reflections
4124 reflections with I > 2σ(I)
R_{	ext{int}} = 0.021

Refinement

R[F^2 > 2σ(F^2)] = 0.037
wR(F^2) = 0.090
S = 1.05
4868 reflections

Table 1

Hydrogen-bond geometry (Å, °).

D—H···A D—H H···A D···A D—H···A
C38—H21C···Cg 0.98 2.61 3.461 (2) 145

Symmetry code: (i) x, −y + ½, z + ½

Data collection: COLLECT (Nonius, 1998); cell refinement: HKLSCALEPACK (Otwinowski & Minor, 1997); data reduction: HKLDENZO (Otwinowski & Minor, 1997) and SCALEPACK; program(s) used to solve structure: SIR92 (Altomare et al., 1994); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997); software used to prepare material for publication: WinGX (Farrugia, 1999), MarvinSketch (Chemaxon, 2010) and publCIF (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2516).

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Dimethyl DL-2,3-dibenzyl-2,3-diisothiocyanatosuccinate

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S1. Comment

The title compound was synthesized as a part of a larger project focusing on the synthesis of 2,3-disubstituted 2,3-di-aminosuccinic acid derivatives obtained from titanium (IV) enolates of 2-isothiocyanato-carboxylates via C—C bond formation in oxidative homo-coupling of titanium (IV) enolates of 2-isothiocyanato-carboxylic esters (Cież, 2007; Cież et al., 2008). The main reason for the interest in vicinal diisothiocyanates is related to their wide application in organic syntheses (Morel & Marchand, 2001). The molecule, crystal structure of which is presented here, belongs to the rare class of organic compounds.

The overall shape of the title molecule is shown in Figure 1. There is pseudo-symmetry in the molecule (2-fold axis perpendicular to C2—C3 bond and parallel to [212]). The mutual orientation of both isothiocyanate groups, same as both benzyl groups, is gauche with dihedral angels N1—C2—C3—N2 = 73.95 (13)° and C21—C2—C3—C31 = 43.41 (16)°. The ester groups are oriented in anti conformation with dihedral angle C1—C2—C3—C4 = 158.31 (11)°.

There are two chiral centres in the molecule, localized on atoms C2 and C3, both with the same absolute configuration (R,R enantiomer shown in Figure 1).

The crystal structure of the title compound is stabilized by weak interactions. The strongest are C—H···π interactions (Arunan et al., 2011a; Arunan et al., 2011b; Malone et al., 1997). They are formed between molecules related via glide plane e. The distance between hydrogen atom and centroid of the aromatic ring (Cg) is 2.611Å, with angle C38—H···Cg = 145.17°. The additionally defined angle of approach of the vector HCg to the plane of the aromatic ring, θ = 77°, and horizontal distance 0.6Å, classify this C—H···π as the second common geometry for this type of interaction observed in crystal structures (type III according to Malone et al., 1997). Intermolecular C—H···π interactions between neighbouring molecules observed in this structure form a zigzag-like chain in the [001] direction (Figure 2), where only one aromatic ring of the title molecule is involved.

Additional interaction is observed between C31—H···O4i [where (i) is x, -y + 1/2, z + 1/2] with C···O = 2.985 (2)Å, H···O = 2.612Å and angle C—H···O = 102.35°. The parameter suggests that it is not a hydrogen bond (Arunan et al., 2011a; Arunan et al., 2011b), however this interaction plays a crucial role in the stabilization of the methyl group (C38), allowing for above mentioned C—H···π. What is interesting, the sulphur atoms of the thiocyanate groups are not involved in intermolecular interactions.

The second aromatic moiety of the DL-2,3-dibenzyl-2,3-diisothiocyanato-succinic acid dimethyl ester is not involved in C—H···π. It is placed in short distance to a corresponding ring of the neighbouring molecule, related via the inversion centre (C24···C24ii = 3.390 (2)Å, where (ii) is -x + 2, -y, -z + 2). However, the overlapping of the aromatic rings is not observed. This suggests a hydrophobic association.
S2. Experimental
The title compound was obtained by oxidative homo-coupling of methyl (S)-2-isothiocyanato-3-phenyl-propionate in TiCl₄/DIEA (N,N-diisopropylethylamine) system at 177 K and characterized by NMR spectroscopy (Cież, 2007). Colourless, block single crystals suitable for X-ray diffraction were obtained from ethanol solution by slow evaporation of solvent at ambient conditions.

S3. Refinement
All non-hydrogen atoms were refined anisotropically using weighted full-matrix least-squares on F². All hydrogen atoms were calculated at idealized positions and refined using a riding model with C—H = 0.95Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic hydrogen atoms, C—H = 0.99Å and U_{iso}(H) = 1.2U_{eq}(C) for methylene groups, C—H = 0.98Å and U_{iso}(H) = 1.5U_{eq}(C) for the methyl groups refined as rotating group.

Figure 1
Asymmetric unit of the title compound - here R,R - enantiomer, showing the molecule conformation. Atom displacement ellipsoids drawn at the 30% probability level and H atoms are shown as spheres of arbitrary radii.
Figure 2
Chain formed by C—H···π interacting molecules, propagating in the [001] direction.

Dimethyl 2,3-dibenzyl-2,3-diisothiocyanatobutanedioate

Crystal data

\[
\begin{align*}
C_{22}H_{20}N_{2}O_{4}S_{2} & \quad F(000) = 920 \\
M_r & = 440.52 \\
Monoclinic, P2_1/c & \quad D_x = 1.353 \text{ Mg m}^{-3} \\
Hall symbol: -P 2ybc & \quad \text{Melting point: } 405(1) \text{ K} \\
a = 9.1658 (1) \text{ Å} & \quad \theta = 1.0–27.5^\circ \\
b = 19.3999 (4) \text{ Å} & \quad \mu = 0.28 \text{ mm}^{-1} \\
c = 12.2762 (2) \text{ Å} & \quad T = 100 \text{ K} \\
\beta = 97.891 (1)^\circ & \quad \text{Block, colourless} \\
V = 2162.23 (6) \text{ Å}^3 & \quad 0.28 \times 0.18 \times 0.18 \text{ mm} \\
Z = 4 & \\
\end{align*}
\]

Data collection

| Nonius KappaCCD diffactometer | 9175 measured reflections |
| Radiation source: fine-focus sealed tube | 4868 independent reflections |
| Graphite monochromator | 4124 reflections with \( I > 2\sigma(I) \) |
| Detector resolution: 9 pixels mm\(^{-1}\) | |
| CCD scans | |
| Absorption correction: multi-scan | |
| (DENZO-SMN; Otwinowski & Minor, 1997) | |
| \( T_{\text{min}} = 0.926, T_{\text{max}} = 0.952 \) | |

Refinement

| Refinement on \( F^2 \) | 0 restraints |
| Least-squares matrix: full | H-atom parameters constrained |
| \( R[F^2 > 2\sigma(F^2)] = 0.037 \) | |
| \( wR^2(F^2) = 0.090 \) | \( w = 1/[\sigma^2(F_o^2) + (0.033P)^2 + 1.1739P] \) |
| \( S = 1.05 \) | where \( P = (F_o^2 + 2F_c^2)/3 \) |
| 4868 reflections | (\( \Delta \sigma \))\(_{\text{max}} \) = 0.001 |
| 273 parameters | \( \Delta\rho_{\text{max}} = 0.35 \text{ e Å}^{-3} \) |
| | \( \Delta\rho_{\text{min}} = -0.52 \text{ e Å}^{-3} \) |

Special details

| Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'s involving l.s. planes. |
| Refinement. Refinement of \( F^2 \) against ALL reflections. The weighted R-factor \( wR \) and goodness of fit \( S \) are based on \( F^2 \), conventional R-factors \( R \) are based on \( F \), with \( F \) set to zero for negative \( F^2 \). The threshold expression of \( F^2 > \sigma(F^2) \) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on \( F^2 \) are statistically about twice as large as those based on \( F \), and R- factors based on ALL data will be even larger. |

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

|  |  |  |  |  |
|---|---|---|---|---|
| S1 | 0.82190 (5) | 0.10092 (2) | 0.64722 (4) | 0.03234 (12) |
| S2 | 0.70194 (5) | 0.41656 (2) | 0.81742 (4) | 0.03349 (12) |
| O1 | 0.77379 (11) | 0.19649 (6) | 1.07866 (8) | 0.0215 (2) |

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| Atom | x     | y     | z     | U(eq) |
|------|-------|-------|-------|-------|
| O3   | 0.32504 (11) | 0.16901 (6) | 0.82274 (8) | 0.0220 (2) |
| O2   | 0.89922 (11) | 0.18316 (6) | 0.93462 (9) | 0.0259 (2) |
| O4   | 0.37916 (13) | 0.26642 (6) | 0.73636 (9) | 0.0296 (3) |
| N1   | 0.65160 (13) | 0.15011 (6) | 0.79822 (10) | 0.0194 (3) |
| N2   | 0.62380 (14) | 0.28759 (7) | 0.88116 (11) | 0.0255 (3) |
| C1   | 0.78640 (15) | 0.18306 (7) | 0.97396 (12) | 0.0183 (3) |
| C22  | 0.65775 (15) | 0.03661 (7) | 0.95391 (12) | 0.0186 (3) |
| C2   | 0.63324 (15) | 0.16521 (7) | 0.91079 (11) | 0.0161 (3) |
| C23  | 0.77233 (16) | 0.01718 (8) | 1.03430 (14) | 0.0259 (3) |
| H4   | 0.799 | 0.0459 | 1.0965 | 0.031* |
| C3   | 0.53140 (15) | 0.23112 (7) | 0.90468 (12) | 0.0179 (3) |
| C29  | 0.73140 (16) | 0.12822 (7) | 0.73867 (12) | 0.0199 (3) |
| C34  | 0.29415 (19) | 0.42686 (8) | 0.98493 (14) | 0.0297 (4) |
| H16  | 0.3257 | 0.4735 | 0.993 | 0.036* |
| C38  | 0.19183 (17) | 0.15756 (10) | 0.74522 (13) | 0.0313 (4) |
| H21A | 0.1091 | 0.1818 | 0.7708 | 0.047* |
| H21B | 0.1704 | 0.1081 | 0.7401 | 0.047* |
| H21C | 0.2065 | 0.1751 | 0.6726 | 0.047* |
| C31  | 0.46259 (15) | 0.24680 (7) | 1.01067 (11) | 0.0184 (3) |
| H13A | 0.4134 | 0.2048 | 1.0336 | 0.022* |
| H13B | 0.5417 | 0.2594 | 1.0706 | 0.022* |
| C35  | 0.14653 (19) | 0.41193 (9) | 0.95249 (14) | 0.0299 (4) |
| H17  | 0.0771 | 0.4482 | 0.9375 | 0.036* |
| C32  | 0.35185 (15) | 0.30495 (7) | 0.99304 (11) | 0.0178 (3) |
| C4   | 0.40438 (16) | 0.22487 (8) | 0.80839 (11) | 0.0199 (3) |
| C21  | 0.57050 (15) | 0.10158 (7) | 0.96548 (12) | 0.0170 (3) |
| H2A  | 0.5699 | 0.1113 | 1.0446 | 0.02* |
| H2B  | 0.4673 | 0.0941 | 0.9317 | 0.02* |
| C36  | 0.10069 (17) | 0.34392 (9) | 0.94210 (12) | 0.0252 (3) |
| H18  | −0.0006 | 0.3336 | 0.9211 | 0.03* |
| C28  | 0.90829 (16) | 0.21203 (9) | 1.15173 (13) | 0.0257 (3) |
| H10A | 0.962 | 0.1692 | 1.1718 | 0.039* |
| H10B | 0.8836 | 0.2345 | 1.2183 | 0.039* |
| H10C | 0.97 | 0.2429 | 1.1144 | 0.039* |
| C27  | 0.62157 (19) | −0.00584 (8) | 0.86285 (14) | 0.0267 (3) |
| H8   | 0.5444 | 0.0072 | 0.8069 | 0.032* |
| C33  | 0.39630 (17) | 0.37363 (8) | 1.00568 (12) | 0.0227 (3) |
| H15  | 0.497 | 0.3842 | 1.0286 | 0.027* |
| C25  | 0.8090 (2) | −0.08616 (9) | 0.93408 (19) | 0.0419 (5) |
| H6   | 0.8596 | −0.1284 | 0.9281 | 0.05* |
| C39  | 0.65003 (16) | 0.34293 (8) | 0.85183 (12) | 0.0202 (3) |
| C26  | 0.6972 (2) | −0.06717 (9) | 0.85291 (17) | 0.0390 (4) |
| H7   | 0.6718 | −0.0959 | 0.7905 | 0.047* |
| C37  | 0.20244 (16) | 0.29063 (8) | 0.96224 (12) | 0.0208 (3) |
| H19  | 0.1701 | 0.2441 | 0.955 | 0.025* |
| C24  | 0.84797 (18) | −0.04410 (9) | 1.02404 (17) | 0.0371 (4) |
| H5   | 0.9265 | −0.057 | 1.079 | 0.045* |
### Atomic displacement parameters (Å²)

|   | $U_{11}$       | $U_{22}$       | $U_{33}$       | $U_{12}$       | $U_{13}$       | $U_{23}$       |
|---|----------------|----------------|----------------|----------------|----------------|----------------|
| S1| 0.0265 (2)     | 0.0405 (3)     | 0.0326 (2)     | −0.00216 (17)  | 0.01345 (16)   | −0.01572 (18)  |
| S2| 0.0424 (2)     | 0.0188 (2)     | 0.0414 (2)     | −0.00374 (17)  | 0.01371 (19)   | 0.00715 (17)   |
| O1| 0.0172 (5)     | 0.0254 (6)     | 0.0216 (5)     | −0.0007 (4)    | 0.0019 (4)     | −0.0027 (4)    |
| O3| 0.0183 (5)     | 0.0277 (6)     | 0.0195 (5)     | 0.0007 (4)     | 0.0004 (4)     | 0.0027 (4)     |
| O2| 0.0178 (5)     | 0.0301 (6)     | 0.0311 (6)     | −0.0020 (4)    | 0.0084 (4)     | −0.0050 (5)    |
| O4| 0.0438 (7)     | 0.0274 (6)     | 0.0182 (5)     | 0.0100 (5)     | 0.0060 (5)     | 0.0058 (4)     |
| N1| 0.0202 (6)     | 0.0190 (6)     | 0.0200 (6)     | 0.0020 (5)     | 0.0058 (5)     | 0.0003 (5)     |
| N2| 0.0267 (7)     | 0.0176 (7)     | 0.0352 (7)     | 0.0015 (5)     | 0.0146 (6)     | 0.0034 (5)     |
| C1| 0.0192 (7)     | 0.0144 (7)     | 0.0227 (7)     | 0.0003 (5)     | 0.0048 (5)     | −0.0003 (5)    |
| C22| 0.0165 (6)    | 0.0147 (6)     | 0.0351 (9)     | 0.0000 (5)     | 0.0094 (5)     | 0.0032 (5)     |
| C2| 0.0170 (6)     | 0.0147 (6)     | 0.0175 (6)     | 0.0011 (5)     | 0.0058 (5)     | −0.0001 (5)    |
| C23| 0.0186 (7)    | 0.0245 (8)     | 0.0353 (9)     | 0.0010 (6)     | 0.0063 (6)     | 0.0100 (6)     |
| C3| 0.0184 (6)     | 0.0147 (6)     | 0.0219 (7)     | 0.0008 (5)     | 0.0076 (5)     | 0.0022 (5)     |
| C29| 0.0188 (7)    | 0.0183 (7)     | 0.0224 (7)     | −0.0028 (6)    | 0.0021 (6)     | −0.0016 (5)    |
| C34| 0.0368 (9)    | 0.0180 (7)     | 0.0361 (9)     | 0.0048 (7)     | 0.0119 (7)     | 0.0001 (6)     |
| C38| 0.0202 (7)    | 0.0512 (11)    | 0.0207 (7)     | 0.0038 (7)     | −0.0039 (6)    | 0.0031 (7)     |
| C31| 0.0192 (7)    | 0.0186 (7)     | 0.0183 (7)     | 0.0030 (5)     | 0.0058 (5)     | −0.0003 (5)    |
| C35| 0.0323 (8)    | 0.0281 (9)     | 0.0303 (8)     | 0.0149 (7)     | 0.0075 (7)     | 0.0046 (7)     |
| C32| 0.0205 (7)    | 0.0181 (7)     | 0.0156 (6)     | 0.0035 (5)     | 0.0053 (5)     | −0.0005 (5)    |
| C4| 0.0240 (7)    | 0.0207 (7)     | 0.0165 (7)     | 0.0075 (6)     | 0.0083 (5)     | 0.0011 (5)     |
| C21| 0.0151 (6)    | 0.0139 (6)     | 0.0227 (7)     | −0.0004 (5)    | 0.0052 (5)     | 0.0018 (5)     |
| C36| 0.0207 (7)    | 0.0344 (9)     | 0.0205 (7)     | 0.0076 (6)     | 0.0029 (6)     | −0.0003 (6)    |
| C28| 0.0173 (7)    | 0.0307 (9)     | 0.0279 (8)     | −0.0013 (6)    | −0.0017 (6)    | −0.0068 (6)    |
| C27| 0.0333 (8)    | 0.0177 (7)     | 0.0308 (8)     | −0.0034 (6)    | 0.0105 (7)     | −0.0008 (6)    |
| C33| 0.0237 (7)    | 0.0200 (7)     | 0.0254 (7)     | 0.0007 (6)     | 0.0071 (6)     | −0.0034 (6)    |
| C25| 0.0413 (10)   | 0.0184 (8)     | 0.0743 (14)    | 0.0109 (7)     | 0.0379 (10)    | 0.0125 (9)     |
| C39| 0.0210 (7)    | 0.0205 (7)     | 0.0195 (7)     | 0.0025 (6)     | 0.0048 (5)     | 0.0001 (6)     |
| C26| 0.0543 (12)   | 0.0188 (8)     | 0.0510 (11)    | −0.0039 (8)    | 0.0326 (10)    | −0.0049 (7)    |
| C37| 0.0214 (7)    | 0.0227 (7)     | 0.0187 (7)     | 0.0012 (6)     | 0.0050 (5)     | −0.0025 (5)    |
| C24| 0.0212 (8)    | 0.0314 (9)     | 0.0616 (12)    | 0.0088 (7)     | 0.0159 (8)     | 0.0240 (9)     |

### Geometric parameters (Å, °)

|   |           |           |           |           |           |           |
|---|-----------|-----------|-----------|-----------|-----------|-----------|
| S1—C29 & 1.5762 (15) | C38—H21B & 0.98 |
| S2—C39 & 1.5813 (15) | C38—H21C & 0.98 |
| O1—C1 & 1.3320 (17) | C31—C32 & 1.5132 (19) |
| O1—C28 & 1.4531 (17) | C31—H13A & 0.99 |
| O3—C4 & 1.3302 (18) | C31—H13B & 0.99 |
| O3—C38 & 1.4583 (17) | C35—C36 & 1.385 (2) |
| O2—C1 & 1.1998 (17) | C35—H17 & 0.95 |
| O4—C4 & 1.1955 (18) | C32—C33 & 1.396 (2) |
| N1—C29 & 1.1818 (19) | C32—C37 & 1.398 (2) |
| N1—C2 & 1.4449 (17) | C21—H2A & 0.99 |
| N2—C39 & 1.168 (2) | C21—H2B & 0.99 |
| N2—C3 & 1.4380 (19) | C36—C37 & 1.392 (2) |
| Bond          | Distance (Å) | Bond          | Distance (Å) |
|--------------|--------------|--------------|--------------|
| C1—C2        | 1.5470 (19)  | C36—H18      | 0.95         |
| C22—C23      | 1.391 (2)    | C28—H10A     | 0.98         |
| C22—C27      | 1.391 (2)    | C28—H10B     | 0.98         |
| C22—C21      | 1.5099 (19)  | C28—H10C     | 0.98         |
| C2—C21       | 1.5528 (19)  | C27—C26      | 1.391 (2)    |
| C2—C3        | 1.5788 (19)  | C27—H8       | 0.95         |
| C23—C24      | 1.391 (2)    | C33—H15      | 0.95         |
| C23—H4       | 0.95         | C25—C26      | 1.378 (3)    |
| C3—C4        | 1.546 (2)    | C25—C24      | 1.380 (3)    |
| C3—C31       | 1.5520 (19)  | C25—H6       | 0.95         |
| C34—C35      | 1.388 (2)    | C26—H7       | 0.95         |
| C34—C33      | 1.394 (2)    | C37—H19      | 0.95         |
| C34—H16      | 0.95         | C24—H5       | 0.95         |
| C38—H21A     | 0.95         |               |              |
| C1—O1—C28    | 117.23 (11)  | C36—C35—H17  | 120.1        |
| C4—O3—C38    | 117.49 (12)  | C34—C35—H17  | 120.1        |
| C29—N1—C2    | 145.87 (13)  | C33—C32—C37  | 118.70 (13)  |
| C39—N2—C3    | 156.08 (15)  | C33—C32—C31  | 121.06 (13)  |
| O2—C1—O1     | 125.58 (13)  | C37—C32—C31  | 120.23 (13)  |
| O2—C1—C2     | 124.86 (13)  | O4—C4—O3     | 126.41 (14)  |
| O1—C1—C2     | 109.54 (11)  | O4—C4—C3     | 124.16 (14)  |
| C23—C22—C27  | 118.89 (14)  | O3—C4—C3     | 109.32 (11)  |
| C23—C22—C21  | 121.17 (14)  | C22—C21—C2   | 112.99 (11)  |
| C27—C22—C21  | 119.92 (13)  | C22—C21—H2A  | 109          |
| N1—C2—C1     | 107.94 (11)  | C22—C21—H2B  | 109          |
| N1—C2—C21    | 110.55 (11)  | C22—C21—H2B  | 109          |
| C1—C2—C21    | 109.01 (11)  | C2—C21—H2B   | 109          |
| N1—C2—C3     | 105.34 (11)  | H2A—C21—H2B  | 107.8        |
| C1—C2—C3     | 109.42 (11)  | C35—C36—H18  | 119.9        |
| C21—C2—C3    | 114.38 (11)  | C37—C36—H18  | 119.9        |
| C24—C23—C22  | 120.31 (17)  | O1—C28—H10A  | 109.5        |
| C24—C23—H4   | 119.8        | O1—C28—H10B  | 109.5        |
| C22—C23—H4   | 119.8        | H10A—C28—H10B| 109.5        |
| N2—C3—C4     | 107.98 (12)  | O1—C28—H10C  | 109.5        |
| N2—C3—C31    | 109.72 (12)  | H10A—C28—H10C| 109.5        |
| C4—C3—C31    | 107.84 (11)  | H10B—C28—H10C| 109.5        |
| N2—C3—C2     | 105.42 (11)  | H10B—C28—H10C| 109.5        |
| C4—C3—C2     | 110.55 (11)  | C26—C27—C22  | 120.68 (17)  |
| C31—C3—C2    | 115.12 (11)  | C26—C27—H8   | 119.7        |
| N1—C29—S1    | 172.86 (14)  | C22—C27—H8   | 119.7        |
| C35—C34—C33  | 120.13 (15)  | C34—C33—C32  | 120.57 (15)  |
| C35—C34—H16  | 119.9        | C34—C33—H15  | 119.7        |
| C33—C34—H16  | 119.9        | C32—C33—H15  | 119.7        |
| O3—C38—H21A  | 109.5        | C26—C25—C24  | 120.37 (16)  |
| O3—C38—H21B  | 109.5        | C26—C25—H6   | 119.8        |
| H21A—C38—H21B| 109.5        | C24—C25—H6   | 119.8        |
| O3—C38—H21C  | 109.5        | N2—C39—S2    | 174.30 (14)  |
Hydrogen-bond geometry (Å, °)

Cg is the centroid of the C32–C37 ring.

|          | D—H  | H···A  | D···A  | D—H···A |
|----------|------|--------|--------|---------|
| C38—H21C···Cg^i | 0.98 | 2.61   | 3.461 (2) | 145 |

Symmetry code: (i) x, −y+1/2, z+1/2.