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3-({[Bis(2-methylpropyl)carbamothioyl]-amino}carbonyl)benzamide

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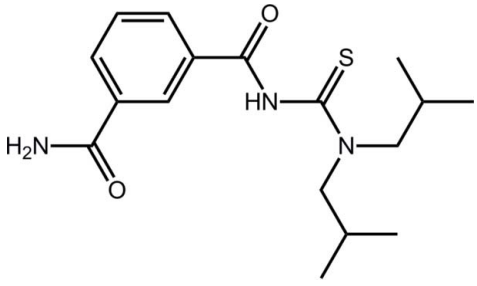
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.039; wR factor = 0.097; data-to-parameter ratio = 18.4.

In the title compound, $C_{17}H_{25}N_3O_2S$, the terminal and central amide groups are, respectively, twisted and coplanar with the attached benzene ring [O—C—C—C torsion angles = 22.7 (3) and 5.4 (3)°]. In the central part of the molecule, the amide and thioamide residues are approximately perpendicular [C—N—C—S torsion angle = −104.98 (18)°]. Supramolecular layers with a zigzag topology are formed in the crystal packing by N—H···O, N—H···S and C—H···O interactions; these stack along c, being separated by hydrophobic interactions.

Related literature

For the preparation of bipodal acylthiourea derivatives, see: Bourne *et al.* (2005). For a related structure, see: Selvakumaran *et al.* (2013).



Experimental

Crystal data

$C_{17}H_{25}N_3O_2S$
M_r = 335.46
Orthorhombic, $P2_12_12$
a = 13.9870 (4) Å
b = 15.7103 (4) Å
c = 8.5532 (3) Å
V = 1879.48 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.18 mm^{-1}
T = 100 K
0.40 × 0.30 × 0.20 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2013)
T_{min} = 0.930, T_{max} = 0.964
6635 measured reflections
4007 independent reflections
3694 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.097
S = 1.00
4007 reflections
218 parameters
30 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}
Absolute structure: Flack (1983), 1590 Friedel pairs
Flack parameter: −0.03 (8)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H12···O2^{i}	0.88	2.09	2.887 (2)	150
N2—H2···O1^{ii}	0.88	1.97	2.797 (2)	155
N1—H11···S1^{ii}	0.88	2.54	3.3908 (18)	163
C7—H7···O1^{ii}	0.95	2.32	3.210 (2)	155

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

Data collection: *CrysAlis PRO* (Agilent, 2013); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG5326).

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3-({[Bis(2-methylpropyl)carbamothioyl]amino}carbonyl)benzamide

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S1. Comment

The title compound, (I), was obtained as a by-product in an attempt to prepare a bipodal acylthiourea derivative (Bourne *et al.*, 2005) from diisobutylamine, isophthaloyl dichloride and potassium thiocyanate in acetone. Crystals were grown from a solution of the compound in acetonitrile/dimethyl formamide mixture (1:1). In (I), Fig. 1, the terminal [O1—C1—C2—C7 torsion angle = 22.7 (3)°] and central [C5—C6—C8—O2 = 5.4 (3)°] amide substituents are twisted and co-planar with the attached benzene ring, respectively. A twist is also noted between the amide and adjacent thioamide residues as seen in the C8—N2—C9—S1 torsion angle of -104.98 (18)°. The methylpropyl substituents lie to either side and are approximately perpendicular to the C_3N plane with the C9—N3—C10—C11/C11′ (50:50 disorder in the iso-propyl group) torsion angles being 126.0 (3) and 87.5 (3)°, respectively, and 100.4 (2)° for C9—N3—C14—C1. The aforementioned conformation matches that found in the accompanying paper (Selvakumaran *et al.*, 2013). In the crystal packing, supramolecular layers with a zigzag topology are formed by N—H···O, N—H···S and C—H···O interactions, Fig. 2 and Table 1. Layers stack along the *c* axis being separated by hydrophobic intertactions.

S2. Experimental

Isophthaloyl dichloride (2.0302 g, 10 mmol) dissolved in acetone (80 ml), was placed in a dropping funnel and added drop wise with stirring to potassium thiocyanate (1.9436 g, 20 mmol) dissolved in acetone (80 ml), under N_2 atmosphere, in a three-necked round bottom flask. The mixture was heated to reflux for 30 minutes and then allowed to cool. A solution of diisobutylamine (2.2850 g, 20 mmol) in acetone (80 ml) was added drop wise from a dropping funnel to the reaction mixture and the resulting mixture was stirred for 2 h at room temperature. Then, hydrochloric acid (0.1 N, 300 ml) was added and the resulting white solid was filtered off, washed with water and dried *in vacuo*. Single crystals were grown at room temperature from acetonitrile/dimethyl formamide mixture (1:1) F T—IR (KBr): $\nu(NH_2)$ 3217 & 3192, ν(N—H) 3405, ν(C═O) 1671 (with adjacent NH_2), ν(C═O) 1652 (with adjacent NH), ν(C═C) 1593, ν(C═S) 1257 cm^{-1}. UV-Visible (DMF): ν_{max}; 264, 283, 363 nm.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions [C—H = 0.95 to 1.00 Å, U_{iso}(H)= 1.2 to 1.5U_{eq}(C)] and were included in the refinement in the riding model approximation. The amino H-atoms were similarly constrained [N—H = 0.88 Å, and with U_{iso}(H)= 1.2U_{eq}(N)]. One isopropyl arm is disordered; the disorder refined to exactly 0.5. The 1,2-related distances were restrained to 1.54±0.01 Å and the 1,3-related ones to 2.51±0.01 Å. The anisotropic displacement parameters of the primed atoms were set to those of the unprimed ones, and the anisotropic displacement parameters were restrained to be nearly isotropic.

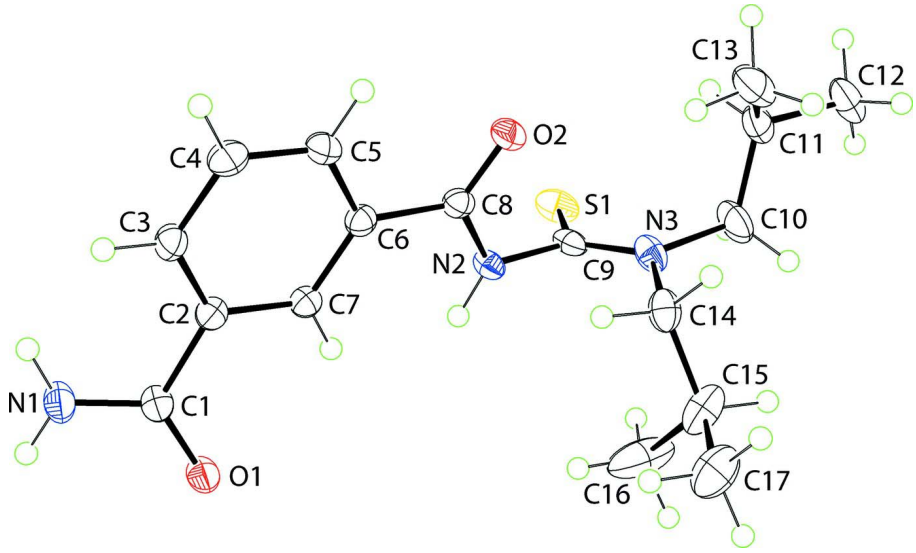

Figure 1

Molecular structure of (I) showing atom-labelling scheme and displacement ellipsoids at the 50% probability level.

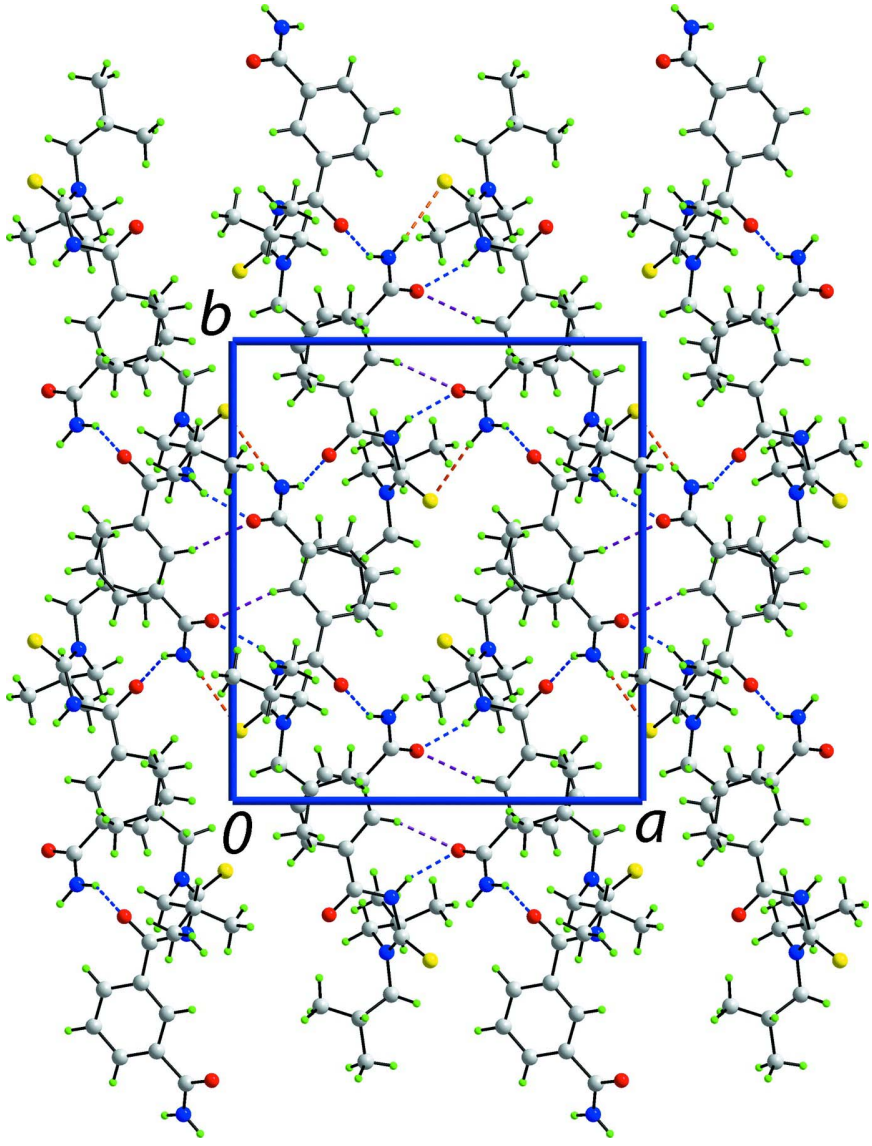

Figure 2

A plan view of the zigzag supramolecular layer in (I). The N—H···O, N—H···S and C—H···O interactions are shown as blue, orange and purple dashed lines, respectively.

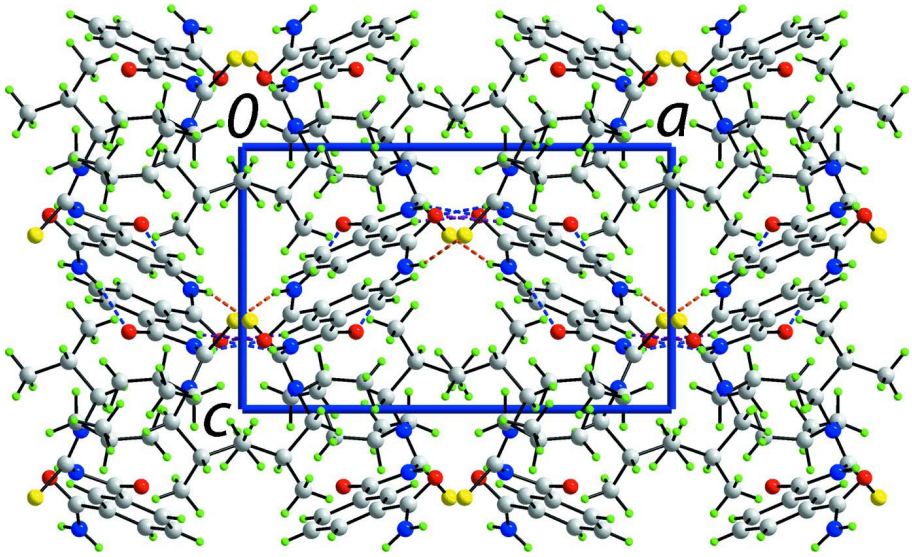

Figure 3

A view of the unit-cell contents in projection down the *b* axis in (I). The N—H···O, N—H···S and C—H···O interactions are shown as blue, orange and purple dashed lines, respectively.

3-({[Bis(2-methylpropyl)carbamothioyl]amino}carbonyl)benzamide

Crystal data

$C_{17}H_{25}N_3O_2S$
$M_r = 335.46$
Orthorhombic, $P2_12_12$
Hall symbol: P 2 2ab
$a = 13.9870$ (4) Å
$b = 15.7103$ (4) Å
$c = 8.5532$ (3) Å
$V = 1879.48$ (10) Å^3
$Z = 4$
$F(000) = 720$
$D_x = 1.186$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3818 reflections
$\theta = 2.4$–$29.3°$
$\mu = 0.18$ mm^{-1}
$T = 100$ K
Block, colourless
0.40 × 0.30 × 0.20 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Radiation source: SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 10.4041 pixels mm^{-1}
ω scan
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2013)
$T_{min} = 0.930$, $T_{max} = 0.964$
6635 measured reflections
4007 independent reflections
3694 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.4°$
$h = -17\rightarrow18$
$k = -17\rightarrow20$
$l = -7\rightarrow10$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.097$
$S = 1.00$
4007 reflections
218 parameters
30 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0461P)^2 + 0.7082P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}
Absolute structure: Flack (1983), 1590 Friedel pairs
Absolute structure parameter: −0.03 (8)

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)
S1	0.01768 (4)	0.15262 (3)	0.66311 (7)	0.03126 (14)	
O1	0.05091 (10)	0.60837 (8)	0.73835 (19)	0.0262 (3)	
O2	0.26459 (10)	0.25192 (9)	0.70500 (17)	0.0268 (3)	
N1	0.12011 (13)	0.68211 (11)	0.5438 (2)	0.0311 (4)	
H11	0.0791	0.7243	0.5533	0.037*	
H12	0.1655	0.6846	0.4727	0.037*	
N2	0.11244 (11)	0.28966 (10)	0.7599 (2)	0.0199 (3)	
H2	0.0705	0.3307	0.7742	0.024*	
N3	0.12403 (12)	0.17031 (10)	0.9200 (2)	0.0253 (4)	
C1	0.11351 (14)	0.61468 (12)	0.6368 (2)	0.0222 (4)	
C2	0.18533 (14)	0.54440 (12)	0.6160 (2)	0.0207 (4)	
C3	0.27479 (14)	0.55770 (13)	0.5504 (3)	0.0247 (4)	
H3	0.2921	0.6127	0.5136	0.030*	
C4	0.33900 (16)	0.49082 (14)	0.5385 (3)	0.0299 (5)	
H4	0.4006	0.5001	0.4948	0.036*	
C5	0.31354 (15)	0.41050 (13)	0.5902 (3)	0.0260 (4)	
H5	0.3578	0.3649	0.5817	0.031*	
C6	0.22343 (13)	0.39591 (12)	0.6546 (2)	0.0204 (4)	
C7	0.15980 (13)	0.46342 (12)	0.6693 (2)	0.0196 (4)	
H7	0.0989	0.4545	0.7157	0.024*	
C8	0.20241 (14)	0.30731 (12)	0.7075 (2)	0.0202 (4)	
C9	0.08818 (13)	0.20345 (12)	0.7909 (2)	0.0221 (4)	
C10	0.11303 (17)	0.07868 (12)	0.9522 (3)	0.0371 (6)	
H10A	0.0508	0.0592	0.9102	0.045*	0.500 (4)
H10B	0.1122	0.0697	1.0668	0.045*	0.500 (4)
H10C	0.0696	0.0722	1.0429	0.045*	0.500 (4)
H10D	0.0812	0.0522	0.8611	0.045*	0.500 (4)
C11	0.1901 (3)	0.0265 (3)	0.8831 (6)	0.0295 (8)	0.500 (4)
H11A	0.1766	0.0275	0.7683	0.035*	0.500 (4)
C12	0.1752 (7)	−0.0672 (4)	0.9301 (7)	0.0374 (13)	0.500 (4)
H12A	0.1078	−0.0765	0.9566	0.056*	0.500 (4)
H12B	0.2152	−0.0805	1.0209	0.056*	0.500 (4)
H12C	0.1930	−0.1042	0.8426	0.056*	0.500 (4)
C13	0.2851 (7)	0.0534 (13)	0.895 (3)	0.0506 (12)	0.500 (4)

H13A	0.2886	0.1149	0.8759	0.076*	0.500 (4)
H13B	0.3241	0.0234	0.8175	0.076*	0.500 (4)
H13C	0.3092	0.0409	1.0002	0.076*	0.500 (4)
C11′	0.2013 (3)	0.0304 (3)	0.9852 (6)	0.0295 (8)	0.50
H11′	0.2189	0.0473	1.0942	0.035*	0.500 (4)
C12′	0.1753 (7)	−0.0640 (4)	0.9979 (7)	0.0374 (13)	0.50
H12D	0.1074	−0.0696	1.0237	0.056*	0.500 (4)
H12E	0.2139	−0.0906	1.0801	0.056*	0.500 (4)
H12F	0.1881	−0.0922	0.8978	0.056*	0.500 (4)
C13′	0.2927 (7)	0.0473 (13)	0.889 (3)	0.0506 (12)	0.50
H13D	0.2991	0.1085	0.8696	0.076*	0.500 (4)
H13E	0.2883	0.0172	0.7886	0.076*	0.500 (4)
H13F	0.3485	0.0268	0.9467	0.076*	0.500 (4)
C14	0.16514 (15)	0.22155 (13)	1.0474 (3)	0.0274 (5)	
H14A	0.1832	0.2782	1.0063	0.033*	
H14B	0.2240	0.1935	1.0861	0.033*	
C15	0.09549 (17)	0.23284 (18)	1.1831 (3)	0.0410 (6)	
H15	0.0827	0.1756	1.2298	0.049*	
C16	0.00072 (19)	0.2703 (2)	1.1290 (3)	0.0612 (9)	
H16A	−0.0273	0.2335	1.0486	0.092*	
H16B	0.0116	0.3272	1.0854	0.092*	
H16C	−0.0431	0.2744	1.2181	0.092*	
C17	0.1423 (2)	0.28857 (19)	1.3076 (3)	0.0475 (7)	
H17A	0.2021	0.2622	1.3421	0.071*	
H17B	0.0989	0.2944	1.3971	0.071*	
H17C	0.1557	0.3449	1.2638	0.071*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0270 (3)	0.0254 (2)	0.0414 (3)	−0.0024 (2)	−0.0020 (2)	−0.0130 (2)
O1	0.0196 (6)	0.0223 (7)	0.0367 (9)	0.0022 (6)	0.0062 (6)	0.0054 (6)
O2	0.0231 (7)	0.0245 (7)	0.0329 (9)	0.0073 (6)	0.0058 (6)	0.0032 (6)
N1	0.0249 (9)	0.0254 (8)	0.0431 (12)	0.0041 (7)	0.0082 (8)	0.0128 (8)
N2	0.0163 (7)	0.0166 (7)	0.0268 (9)	0.0017 (6)	0.0003 (7)	−0.0011 (7)
N3	0.0212 (8)	0.0179 (8)	0.0370 (10)	−0.0007 (6)	−0.0017 (7)	0.0028 (7)
C1	0.0179 (9)	0.0216 (9)	0.0272 (11)	−0.0012 (8)	−0.0013 (8)	0.0026 (8)
C2	0.0189 (9)	0.0230 (9)	0.0202 (10)	0.0002 (8)	−0.0005 (7)	0.0013 (8)
C3	0.0226 (9)	0.0235 (9)	0.0280 (11)	−0.0006 (8)	0.0041 (8)	0.0051 (9)
C4	0.0213 (10)	0.0330 (11)	0.0354 (12)	−0.0006 (9)	0.0101 (10)	0.0022 (10)
C5	0.0233 (10)	0.0241 (10)	0.0307 (12)	0.0052 (8)	0.0055 (9)	0.0014 (9)
C6	0.0200 (9)	0.0227 (9)	0.0186 (9)	0.0006 (7)	−0.0002 (8)	0.0008 (8)
C7	0.0176 (8)	0.0218 (9)	0.0196 (9)	−0.0002 (7)	−0.0002 (8)	0.0001 (8)
C8	0.0213 (9)	0.0221 (9)	0.0173 (10)	0.0021 (8)	−0.0012 (7)	−0.0019 (7)
C9	0.0174 (8)	0.0176 (9)	0.0312 (12)	0.0027 (7)	0.0045 (8)	−0.0034 (8)
C10	0.0390 (13)	0.0167 (10)	0.0556 (16)	0.0022 (9)	0.0046 (12)	0.0065 (10)
C11	0.0374 (17)	0.0237 (13)	0.0274 (17)	0.0075 (12)	−0.0093 (16)	0.0005 (16)
C12	0.0503 (17)	0.0218 (13)	0.040 (4)	0.0101 (12)	−0.019 (4)	−0.004 (3)

C13	0.0451 (18)	0.042 (2)	0.065 (2)	0.0223 (19)	0.0127 (18)	0.0127 (18)
C11′	0.0374 (17)	0.0237 (13)	0.0274 (17)	0.0075 (12)	−0.0093 (16)	0.0005 (16)
C12′	0.0503 (17)	0.0218 (13)	0.040 (4)	0.0101 (12)	−0.019 (4)	−0.004 (3)
C13′	0.0451 (18)	0.042 (2)	0.065 (2)	0.0223 (19)	0.0127 (18)	0.0127 (18)
C14	0.0238 (10)	0.0267 (10)	0.0318 (12)	−0.0025 (8)	−0.0064 (9)	0.0066 (9)
C15	0.0399 (13)	0.0582 (16)	0.0249 (12)	−0.0110 (12)	−0.0014 (11)	0.0082 (11)
C16	0.0314 (13)	0.117 (3)	0.0349 (15)	0.0081 (16)	0.0033 (11)	−0.0206 (16)
C17	0.0487 (15)	0.0643 (17)	0.0297 (14)	−0.0072 (13)	−0.0058 (12)	0.0027 (12)

Geometric parameters (Å, º)

S1—C9	1.675 (2)	C11—C13	1.398 (13)
O1—C1	1.237 (2)	C11—C12	1.540 (7)
O2—C8	1.230 (2)	C11—H11A	1.0000
N1—C1	1.328 (3)	C12—H12A	0.9800
N1—H11	0.8800	C12—H12B	0.9800
N1—H12	0.8800	C12—H12C	0.9800
N2—C8	1.364 (2)	C13—H13A	0.9800
N2—C9	1.421 (2)	C13—H13B	0.9800
N2—H2	0.8800	C13—H13C	0.9800
N3—C9	1.320 (3)	C11′—C13′	1.545 (9)
N3—C14	1.472 (3)	C11′—C12′	1.531 (6)
N3—C10	1.474 (2)	C11′—H11′	1.0000
C1—C2	1.503 (3)	C12′—H12D	0.9800
C2—C3	1.387 (3)	C12′—H12E	0.9800
C2—C7	1.398 (3)	C12′—H12F	0.9800
C3—C4	1.386 (3)	C13′—H13D	0.9800
C3—H3	0.9500	C13′—H13E	0.9800
C4—C5	1.384 (3)	C13′—H13F	0.9800
C4—H4	0.9500	C14—C15	1.525 (3)
C5—C6	1.394 (3)	C14—H14A	0.9900
C5—H5	0.9500	C14—H14B	0.9900
C6—C7	1.390 (3)	C15—C17	1.526 (4)
C6—C8	1.493 (3)	C15—C16	1.523 (4)
C7—H7	0.9500	C15—H15	1.0000
C10—C11′	1.475 (4)	C16—H16A	0.9800
C10—C11	1.478 (5)	C16—H16B	0.9800
C10—H10A	0.9900	C16—H16C	0.9800
C10—H10B	0.9900	C17—H17A	0.9800
C10—H10C	0.9900	C17—H17B	0.9800
C10—H10D	0.9900	C17—H17C	0.9800
C1—N1—H11	120.0	C11—C12—H12A	109.5
C1—N1—H12	120.0	C11—C12—H12B	109.5
H11—N1—H12	120.0	H12A—C12—H12B	109.5
C8—N2—C9	118.37 (16)	C11—C12—H12C	109.5
C8—N2—H2	120.8	H12A—C12—H12C	109.5
C9—N2—H2	120.8	H12B—C12—H12C	109.5

C9—N3—C14	123.52 (16)	C11—C13—H13A	109.5
C9—N3—C10	120.15 (19)	C11—C13—H13B	109.5
C14—N3—C10	115.87 (19)	H13A—C13—H13B	109.5
O1—C1—N1	122.25 (18)	C11—C13—H13C	109.5
O1—C1—C2	119.81 (17)	H13A—C13—H13C	109.5
N1—C1—C2	117.94 (18)	H13B—C13—H13C	109.5
C3—C2—C7	119.97 (18)	C10—C11′—C13′	120.2 (8)
C3—C2—C1	122.69 (17)	C10—C11′—C12′	108.2 (4)
C7—C2—C1	117.33 (17)	C13′—C11′—C12′	113.6 (8)
C2—C3—C4	120.00 (19)	C10—C11′—H11′	104.4
C2—C3—H3	120.0	C13′—C11′—H11′	104.4
C4—C3—H3	120.0	C12′—C11′—H11′	104.4
C5—C4—C3	120.08 (19)	C11′—C12′—H12D	109.5
C5—C4—H4	120.0	C11′—C12′—H12E	109.5
C3—C4—H4	120.0	H12D—C12′—H12E	109.5
C4—C5—C6	120.58 (19)	C11′—C12′—H12F	109.5
C4—C5—H5	119.7	H12D—C12′—H12F	109.5
C6—C5—H5	119.7	H12E—C12′—H12F	109.5
C7—C6—C5	119.28 (18)	C11′—C13′—H13D	109.5
C7—C6—C8	123.91 (17)	C11′—C13′—H13E	109.5
C5—C6—C8	116.80 (17)	H13D—C13′—H13E	109.5
C6—C7—C2	120.08 (18)	C11′—C13′—H13F	109.5
C6—C7—H7	120.0	H13D—C13′—H13F	109.5
C2—C7—H7	120.0	H13E—C13′—H13F	109.5
O2—C8—N2	120.92 (18)	N3—C14—C15	112.17 (18)
O2—C8—C6	120.99 (17)	N3—C14—H14A	109.2
N2—C8—C6	118.08 (16)	C15—C14—H14A	109.2
N3—C9—N2	116.19 (17)	N3—C14—H14B	109.2
N3—C9—S1	125.57 (15)	C15—C14—H14B	109.2
N2—C9—S1	118.24 (16)	H14A—C14—H14B	107.9
C11′—C10—N3	116.8 (2)	C14—C15—C17	108.9 (2)
N3—C10—C11	113.0 (2)	C14—C15—C16	111.7 (2)
N3—C10—H10A	109.0	C17—C15—C16	111.3 (2)
C11—C10—H10A	109.0	C14—C15—H15	108.3
N3—C10—H10B	109.0	C17—C15—H15	108.3
C11—C10—H10B	109.0	C16—C15—H15	108.3
H10A—C10—H10B	107.8	C15—C16—H16A	109.5
C11′—C10—H10C	108.1	C15—C16—H16B	109.5
N3—C10—H10C	108.1	H16A—C16—H16B	109.5
C11′—C10—H10D	108.1	C15—C16—H16C	109.5
N3—C10—H10D	108.1	H16A—C16—H16C	109.5
H10C—C10—H10D	107.3	H16B—C16—H16C	109.5
C13—C11—C10	119.7 (9)	C15—C17—H17A	109.5
C13—C11—C12	113.5 (9)	C15—C17—H17B	109.5
C10—C11—C12	109.1 (4)	H17A—C17—H17B	109.5
C13—C11—H11A	104.2	C15—C17—H17C	109.5
C10—C11—H11A	104.2	H17A—C17—H17C	109.5
C12—C11—H11A	104.2	H17B—C17—H17C	109.5

O1—C1—C2—C3	−155.8 (2)	C10—N3—C9—N2	−172.35 (18)
N1—C1—C2—C3	24.2 (3)	C14—N3—C9—S1	−164.30 (16)
O1—C1—C2—C7	22.7 (3)	C10—N3—C9—S1	7.6 (3)
N1—C1—C2—C7	−157.3 (2)	C8—N2—C9—N3	75.0 (2)
C7—C2—C3—C4	−0.3 (3)	C8—N2—C9—S1	−104.98 (18)
C1—C2—C3—C4	178.1 (2)	C9—N3—C10—C11′	126.0 (3)
C2—C3—C4—C5	0.8 (4)	C14—N3—C10—C11′	−61.5 (3)
C3—C4—C5—C6	0.0 (4)	C9—N3—C10—C11	87.5 (3)
C4—C5—C6—C7	−1.2 (3)	C14—N3—C10—C11	−100.0 (3)
C4—C5—C6—C8	−179.8 (2)	C11′—C10—C11—C13	−60.3 (12)
C5—C6—C7—C2	1.7 (3)	N3—C10—C11—C13	44.0 (12)
C8—C6—C7—C2	−179.77 (19)	C11′—C10—C11—C12	72.9 (5)
C3—C2—C7—C6	−1.0 (3)	N3—C10—C11—C12	177.1 (4)
C1—C2—C7—C6	−179.47 (18)	N3—C10—C11′—C13′	−41.3 (10)
C9—N2—C8—O2	−8.7 (3)	C11—C10—C11′—C13′	51.2 (9)
C9—N2—C8—C6	171.83 (18)	N3—C10—C11′—C12′	−174.1 (4)
C7—C6—C8—O2	−173.1 (2)	C11—C10—C11′—C12′	−81.5 (5)
C5—C6—C8—O2	5.4 (3)	C9—N3—C14—C15	100.4 (2)
C7—C6—C8—N2	6.4 (3)	C10—N3—C14—C15	−71.8 (2)
C5—C6—C8—N2	−175.10 (19)	N3—C14—C15—C17	−178.37 (19)
C14—N3—C9—N2	15.8 (3)	N3—C14—C15—C16	−55.0 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H12···O2^{i}	0.88	2.09	2.887 (2)	150
N2—H2···O1^{ii}	0.88	1.97	2.797 (2)	155
N1—H11···S1^{ii}	0.88	2.54	3.3908 (18)	163
C7—H7···O1^{ii}	0.95	2.32	3.210 (2)	155

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