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4-{[4-(3,5-Dimethoxybenzamido)-phenyl]sulfanyl}-*N*-methylpyridine-2-carboxamide

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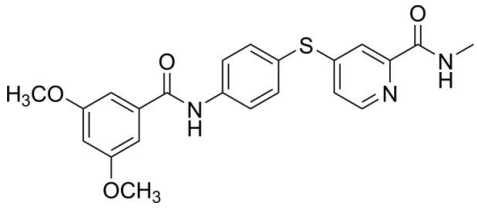
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.044; wR factor = 0.065; data-to-parameter ratio = 16.1.

There are two independent molecules in the asymmetric unit of the title compound, $C_{22}H_{21}N_3O_4S$. The central benzene ring makes dihedral angles of 74.28 (6) and 68.84 (6)° with the pyridine and 3,5-dimethoxyphenyl rings, respectively, in one molecule [86.66 (6) and 81.14 (6)° respectively, in the other]. Each of the molecules forms a centrosymmetric dimer with another molecule *via* pairs of intermolecular N—H···O hydrogen bonds. These hydrogen bonds connect the N—H groups and the O atoms of the carbonyl groups next to the 3,5-dimethoxyphenyl rings. Additional intermolecular N—H···O interactions link the dimers in the crystal structure.

Related literature

For related compounds and their biological activity, see: Khire *et al.* (2004); Dominguez *et al.* (2007).



Experimental

Crystal data

$C_{22}H_{21}N_3O_4S$
M_r = 423.49
Triclinic, $P\overline{1}$
a = 11.1165 (5) Å
b = 13.5678 (6) Å
c = 15.3183 (6) Å
α = 102.723 (4)°
β = 105.949 (4)°
γ = 90.975 (4)°
V = 2159.51 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.18 mm^{-1}
T = 293 K
0.24 × 0.20 × 0.17 mm

Data collection

Oxford Diffraction Xcalibur Eos diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010)
T_{min} = 0.989, T_{max} = 1.0
18448 measured reflections
8806 independent reflections
4117 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.065
S = 1.00
8806 reflections
547 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O4^{i}	0.86	2.12	2.941 (2)	159
N3—H3···O7^{ii}	0.86	2.22	2.922 (2)	138
N4—H4···O8^{iii}	0.86	2.15	2.985 (2)	163
N6—H6···O3^{iv}	0.86	2.30	2.957 (2)	133

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); 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: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2*.

We thank the Analytical and Testing Center of Sichuan University for the X-ray measurements.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2258).

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supporting information

Acta Cryst. (2011). E**67**, o856 [doi:10.1107/S1600536811006490]

4-{[4-(3,5-Dimethoxybenzamido)phenyl]sulfanyl}-*N*-methylpyridine-2-carboxamide

Ting-Ting Huang, Na-Na Meng, Xiao-Yu Qing and Luo-Ting Yu

S1. Comment

Sorafenib is of great importance owing to its antitumor properties (Khire *et al.*, 2004; Dominguez *et al.*, 2007). The title compound, as one of its derivatives, possessed even better *in vitro* anticancer activity against both two tumor cell lines (HCT116 and HEPG2). As a potent antitumor drug, we report here its crystal structure. In the title molecule, $C_{22}H_{21}N_3O_4S$, (Fig. 1), the phenyl ring makes dihedral angles of 78.54 (6)° and 75.30 (6)° with the pyridine ring and the 3,5-dimethoxyphenyl ring, respectively. In crystal, the molecules form centrosymmetric dimers *via* a pair of intermolecular N–H···O hydrogen bonds. In the crystal structure, intermolecular N—H···O hydrogen-bonding interactions between the dimers form an infinite three-dimensional structure (Table 1 and Fig. 2).

S2. Experimental

To the suspension of anhydrous potassium carbonate (0.69 g, 5.00 mmol) and 4-(4-aminophenylthio)-*N*-methyl-picolinamide (0.52 g, 2.00 mmol) in 7.00 ml THF was added dropwise 3,5-dimethoxybenzoyl chloride (0.42 g, 2.10 mmol). After being stirred at room temperature for 2 h, the mixture was extracted with 30 ml e thyl acetate and 30 ml brine for three times and the combined organic layers were dried over anhydrous sodium sulfate. Then the solution was concentrated under vacuum, and the residue was recrystallized from ethanol to give the title compound, with 32.13% yield. Crystals suitable for X-ray analysis were obtained by slow evaporation from an ethanolic solution at room temperature.

S3. Refinement

H atoms at N1 and N3 were located in a difference map and refined isotropically. The remaining H atoms were positioned geometrically (C—H = 0.93–0.96 Å) and refined using a riding model, with U_{iso}(H) = 1.2–1.5 U_{eq}(C).

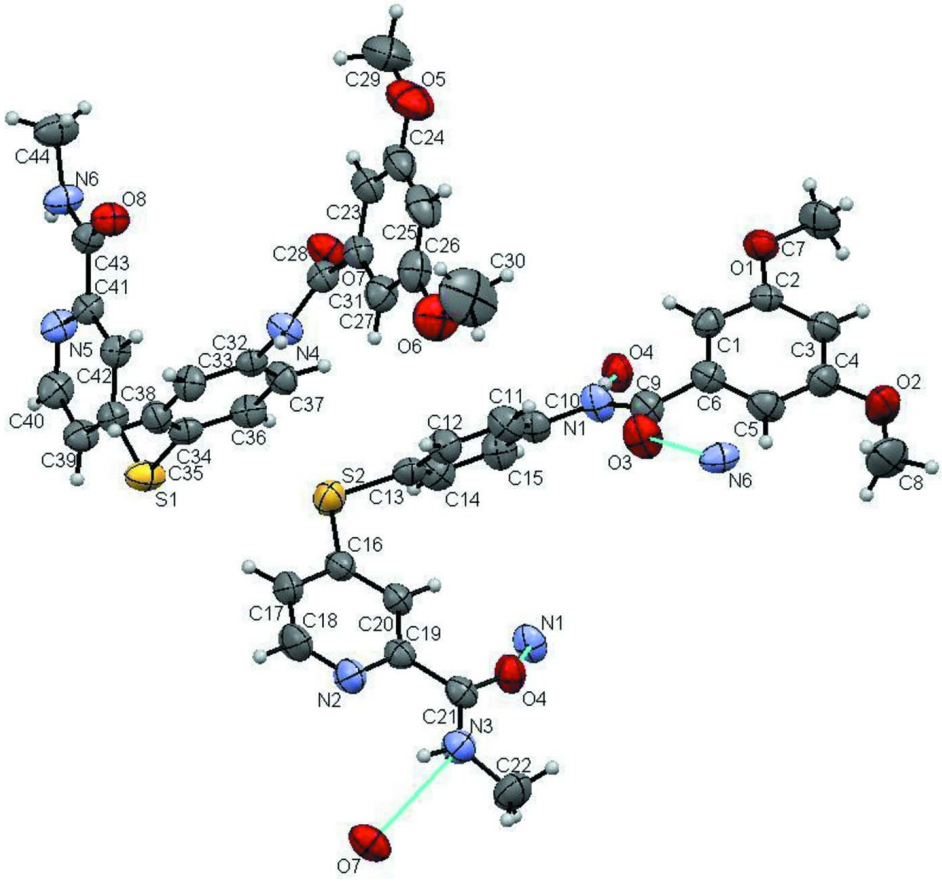

Figure 1

Molecular structure of the title compound with displacement ellipsoids drawn at the 30% probability level.

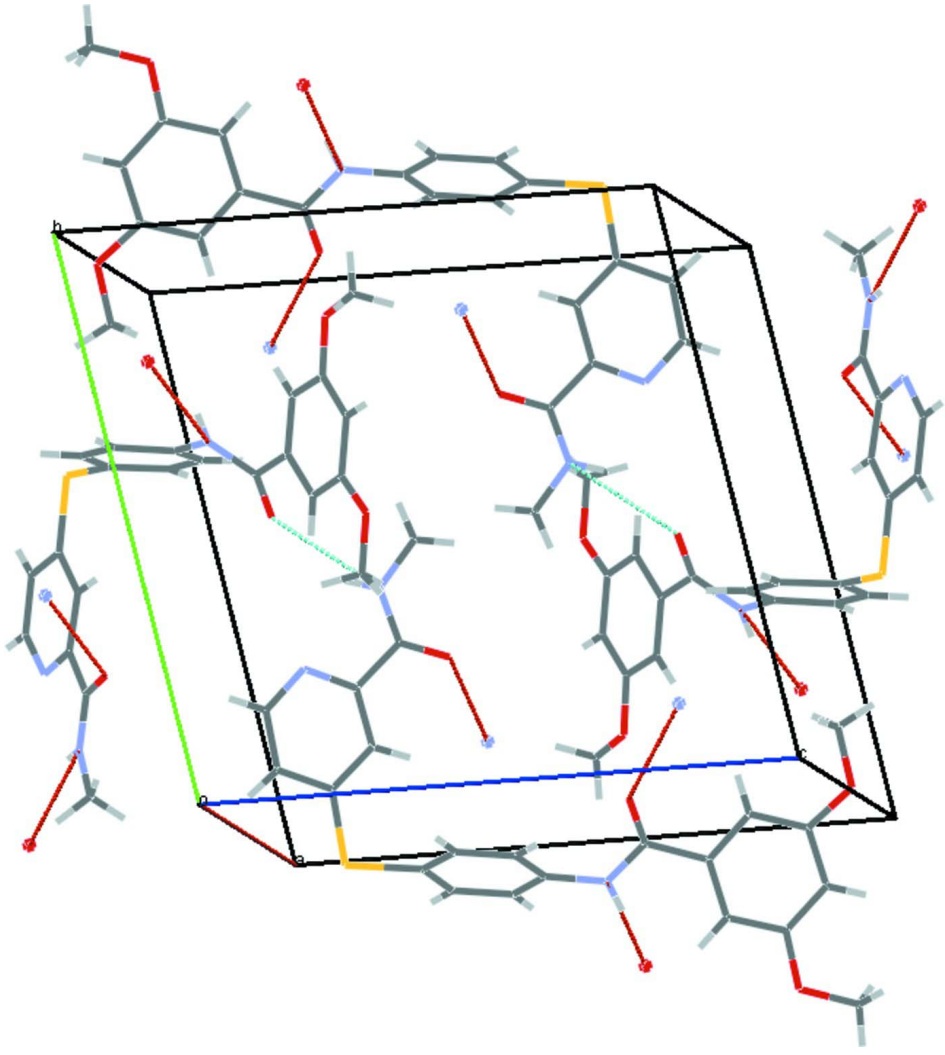

Figure 2

Packing diagram of the title compound.

4-{[4-(3,5-Dimethoxybenzamido)phenyl]sulfanyl}-*N*-methylpyridine- 2-carboxamide

Crystal data

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$M_r = 423.49$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 11.1165\ (5)$ Å
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$c = 15.3183\ (6)$ Å
$\alpha = 102.723\ (4)°$
$\beta = 105.949\ (4)°$
$\gamma = 90.975\ (4)°$
$V = 2159.51\ (16)$ Å^3
$Z = 4$
$F(000) = 888$
$D_x = 1.303$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.7107$ Å
Cell parameters from 5046 reflections
$\theta = 2.9–29.2°$
$\mu = 0.18$ mm^{-1}
$T = 293$ K
Block, orange
0.24 × 0.20 × 0.17 mm

Data collection

Oxford Diffraction Xcalibur Eos diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 16.0874 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010)
T_{min} = 0.989, T_{max} = 1.0

18448 measured reflections
8806 independent reflections
4117 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 26.4°, θ_{min} = 2.9°
h = −13→13
k = −16→16
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.065
S = 1.00
8806 reflections
547 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.0126P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Special details

Experimental. CrysAlisPro, Oxford Diffraction Ltd., Version 1.171.33.66 (release 28-04-2010 CrysAlis171 .NET) (compiled Apr 28 2010,14:27:37) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

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.

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)

	x	y	z	U_{iso}*/U_{eq}
S1	0.65660 (6)	0.37812 (4)	1.12524 (4)	0.05655 (19)
O1	0.39178 (13)	0.32537 (11)	0.17737 (9)	0.0536 (4)
O2	0.33947 (17)	−0.01920 (13)	0.01326 (11)	0.0862 (6)
O3	0.64974 (15)	0.00594 (12)	0.34157 (10)	0.0708 (5)
O4	0.64438 (14)	−0.26093 (10)	0.57675 (10)	0.0568 (4)
N1	0.56894 (16)	0.13586 (12)	0.42239 (12)	0.0541 (5)
H1	0.5175	0.1823	0.4170	0.065*
N2	0.89197 (18)	−0.23172 (14)	0.78726 (14)	0.0582 (5)
N3	0.74299 (16)	−0.37746 (14)	0.64935 (12)	0.0553 (5)
H3	0.8025	−0.3878	0.6951	0.066*
C1	0.48731 (19)	0.20452 (16)	0.25279 (15)	0.0453 (6)
H1A	0.5205	0.2565	0.3056	0.054*
C2	0.4130 (2)	0.22594 (17)	0.17137 (16)	0.0409 (6)

C3	0.3640 (2)	0.14940 (17)	0.09286 (15)	0.0513 (6)
H3A	0.3123	0.1638	0.0389	0.062*
C4	0.3926 (2)	0.05029 (18)	0.09486 (17)	0.0553 (7)
C5	0.4657 (2)	0.02726 (17)	0.17531 (17)	0.0555 (7)
H5	0.4841	−0.0392	0.1764	0.067*
C6	0.5116 (2)	0.10566 (18)	0.25486 (16)	0.0460 (6)
C7	0.3120 (2)	0.35033 (16)	0.09594 (15)	0.0696 (7)
H7B	0.3508	0.3355	0.0462	0.104*
H7C	0.2990	0.4212	0.1096	0.104*
H7A	0.2327	0.3110	0.0773	0.104*
C8	0.3678 (2)	−0.12126 (17)	0.00739 (16)	0.0935 (10)
H8C	0.4572	−0.1244	0.0242	0.140*
H8B	0.3313	−0.1602	−0.0553	0.140*
H8A	0.3342	−0.1485	0.0493	0.140*
C9	0.5843 (2)	0.07740 (18)	0.34252 (16)	0.0508 (6)
C10	0.6310 (2)	0.12627 (15)	0.51350 (16)	0.0461 (6)
C11	0.7543 (2)	0.10139 (15)	0.53712 (16)	0.0557 (7)
H11	0.7976	0.0900	0.4923	0.067*
C12	0.8126 (2)	0.09347 (15)	0.62633 (16)	0.0520 (6)
H12	0.8951	0.0761	0.6413	0.062*
C13	0.7502 (2)	0.11111 (15)	0.69480 (15)	0.0465 (6)
C14	0.6284 (2)	0.13777 (15)	0.67162 (16)	0.0544 (6)
H14	0.5857	0.1508	0.7168	0.065*
C15	0.5693 (2)	0.14532 (15)	0.58157 (16)	0.0551 (6)
H15	0.4871	0.1634	0.5667	0.066*
C16	0.8519 (2)	−0.02610 (16)	0.79660 (15)	0.0460 (6)
C17	0.9419 (2)	−0.05579 (18)	0.86601 (15)	0.0579 (7)
H17	0.9908	−0.0079	0.9174	0.069*
C18	0.9577 (2)	−0.1577 (2)	0.85779 (17)	0.0688 (8)
H18	1.0190	−0.1761	0.9051	0.083*
C19	0.8052 (2)	−0.20169 (17)	0.72111 (15)	0.0430 (6)
C20	0.78341 (19)	−0.10110 (16)	0.72188 (14)	0.0431 (6)
H20	0.7235	−0.0845	0.6728	0.052*
C21	0.7239 (2)	−0.28288 (18)	0.64210 (16)	0.0450 (6)
C22	0.6663 (2)	−0.46444 (16)	0.58221 (16)	0.0773 (8)
H22B	0.5870	−0.4711	0.5949	0.116*
H22C	0.7088	−0.5248	0.5874	0.116*
H22A	0.6526	−0.4546	0.5201	0.116*
S2	0.83017 (6)	0.10378 (4)	0.80987 (4)	0.06080 (19)
O5	1.15357 (17)	0.53884 (17)	0.58562 (12)	0.0965 (6)
O6	1.08908 (16)	0.18987 (14)	0.57927 (12)	0.0908 (6)
O7	0.84584 (14)	0.49944 (11)	0.78247 (10)	0.0623 (5)
O8	0.83861 (13)	0.74737 (10)	1.12151 (10)	0.0537 (4)
N4	0.93679 (14)	0.37157 (11)	0.84322 (11)	0.0444 (5)
H4	0.9932	0.3291	0.8417	0.053*
N5	0.62508 (15)	0.71220 (13)	1.24900 (12)	0.0482 (5)
N6	0.74652 (15)	0.86110 (13)	1.20748 (11)	0.0523 (5)
H6	0.6911	0.8696	1.2376	0.063*

C23	1.03238 (19)	0.48973 (17)	0.68142 (14)	0.0529 (6)
H23	1.0154	0.5559	0.7038	0.063*
C24	1.1014 (2)	0.4680 (2)	0.61764 (17)	0.0623 (7)
C25	1.1221 (2)	0.3681 (2)	0.58183 (15)	0.0676 (8)
H25	1.1677	0.3542	0.5385	0.081*
C26	1.0758 (2)	0.2906 (2)	0.61010 (17)	0.0612 (7)
C27	1.00969 (19)	0.31162 (17)	0.67610 (15)	0.0547 (7)
H27	0.9795	0.2591	0.6964	0.066*
C28	0.98907 (19)	0.40933 (17)	0.71110 (14)	0.0443 (6)
C29	1.1378 (3)	0.6419 (2)	0.61998 (19)	0.1054 (11)
H29A	1.0500	0.6523	0.6043	0.158*
H29B	1.1800	0.6835	0.5924	0.158*
H29C	1.1728	0.6599	0.6866	0.158*
C30	1.1599 (3)	0.1633 (2)	0.51522 (19)	0.1318 (13)
H30A	1.1195	0.1831	0.4585	0.198*
H30B	1.1658	0.0913	0.5019	0.198*
H30C	1.2426	0.1973	0.5417	0.198*
C31	0.9166 (2)	0.43189 (17)	0.78087 (15)	0.0454 (6)
C32	0.8700 (2)	0.37503 (14)	0.91011 (15)	0.0378 (5)
C33	0.93255 (19)	0.36860 (14)	0.99944 (15)	0.0471 (6)
H33	1.0186	0.3627	1.0155	0.057*
C34	0.8686 (2)	0.37083 (14)	1.06550 (14)	0.0488 (6)
H34	0.9121	0.3669	1.1257	0.059*
C35	0.7406 (2)	0.37881 (14)	1.04267 (15)	0.0407 (6)
C36	0.67767 (19)	0.38272 (14)	0.95225 (15)	0.0464 (6)
H36	0.5913	0.3874	0.9357	0.056*
C37	0.7419 (2)	0.37978 (14)	0.88621 (15)	0.0476 (6)
H37	0.6983	0.3810	0.8253	0.057*
C38	0.64704 (18)	0.50777 (15)	1.17087 (13)	0.0402 (6)
C39	0.57828 (19)	0.53448 (17)	1.23420 (15)	0.0491 (6)
H39	0.5380	0.4849	1.2520	0.059*
C40	0.57063 (19)	0.63515 (18)	1.27021 (14)	0.0540 (6)
H40	0.5241	0.6514	1.3127	0.065*
C41	0.69385 (18)	0.68463 (16)	1.18968 (14)	0.0397 (6)
C42	0.70578 (17)	0.58534 (15)	1.14923 (13)	0.0396 (5)
H42	0.7535	0.5708	1.1074	0.047*
C43	0.76637 (19)	0.76806 (17)	1.16986 (15)	0.0433 (6)
C44	0.8143 (2)	0.94991 (15)	1.20025 (15)	0.0692 (8)
H44B	0.8810	0.9292	1.1734	0.104*
H44C	0.8488	0.9933	1.2613	0.104*
H44A	0.7579	0.9859	1.1612	0.104*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0725 (5)	0.0409 (4)	0.0687 (5)	0.0063 (3)	0.0411 (4)	0.0118 (3)
O1	0.0681 (12)	0.0412 (11)	0.0543 (11)	0.0103 (8)	0.0185 (9)	0.0156 (8)
O2	0.1402 (18)	0.0447 (12)	0.0569 (12)	0.0043 (11)	0.0116 (12)	−0.0018 (10)

O3	0.0842 (14)	0.0676 (13)	0.0659 (12)	0.0430 (10)	0.0266 (10)	0.0178 (9)
O4	0.0598 (12)	0.0578 (11)	0.0464 (10)	0.0173 (9)	0.0037 (9)	0.0124 (8)
N1	0.0638 (14)	0.0518 (13)	0.0488 (13)	0.0288 (10)	0.0154 (11)	0.0152 (11)
N2	0.0547 (15)	0.0582 (15)	0.0561 (14)	0.0054 (11)	−0.0018 (12)	0.0238 (12)
N3	0.0542 (14)	0.0488 (14)	0.0595 (14)	0.0101 (11)	0.0065 (11)	0.0175 (11)
C1	0.0493 (16)	0.0411 (16)	0.0460 (15)	0.0011 (12)	0.0184 (13)	0.0056 (12)
C2	0.0459 (16)	0.0332 (16)	0.0488 (16)	0.0037 (12)	0.0204 (13)	0.0118 (13)
C3	0.0671 (18)	0.0427 (17)	0.0466 (16)	0.0053 (13)	0.0183 (14)	0.0132 (13)
C4	0.076 (2)	0.0416 (18)	0.0477 (17)	0.0048 (14)	0.0214 (15)	0.0051 (14)
C5	0.0748 (19)	0.0425 (17)	0.0576 (18)	0.0157 (14)	0.0297 (15)	0.0147 (14)
C6	0.0490 (16)	0.0458 (17)	0.0500 (16)	0.0123 (13)	0.0221 (13)	0.0145 (13)
C7	0.075 (2)	0.0595 (18)	0.0770 (19)	0.0254 (14)	0.0147 (16)	0.0302 (15)
C8	0.154 (3)	0.0420 (19)	0.077 (2)	0.0053 (18)	0.038 (2)	−0.0063 (15)
C9	0.0552 (18)	0.0508 (18)	0.0501 (17)	0.0127 (13)	0.0205 (14)	0.0123 (14)
C10	0.0500 (17)	0.0400 (15)	0.0481 (16)	0.0154 (12)	0.0119 (14)	0.0116 (12)
C11	0.0564 (19)	0.0570 (17)	0.0605 (18)	0.0165 (14)	0.0233 (15)	0.0188 (14)
C12	0.0437 (16)	0.0528 (16)	0.0585 (17)	0.0113 (12)	0.0098 (14)	0.0164 (13)
C13	0.0548 (18)	0.0324 (14)	0.0498 (16)	0.0016 (12)	0.0112 (14)	0.0096 (11)
C14	0.0611 (19)	0.0515 (16)	0.0552 (17)	0.0147 (13)	0.0237 (15)	0.0126 (13)
C15	0.0502 (17)	0.0598 (17)	0.0562 (17)	0.0208 (13)	0.0162 (15)	0.0130 (13)
C16	0.0480 (17)	0.0477 (16)	0.0448 (16)	0.0029 (13)	0.0124 (13)	0.0169 (13)
C17	0.0614 (19)	0.0573 (19)	0.0474 (16)	−0.0049 (14)	−0.0010 (13)	0.0181 (13)
C18	0.065 (2)	0.072 (2)	0.063 (2)	0.0064 (16)	−0.0072 (15)	0.0356 (17)
C19	0.0404 (16)	0.0470 (16)	0.0442 (16)	0.0057 (13)	0.0119 (13)	0.0162 (13)
C20	0.0464 (16)	0.0461 (16)	0.0399 (15)	0.0090 (12)	0.0132 (12)	0.0150 (12)
C21	0.0505 (18)	0.0479 (18)	0.0442 (16)	0.0131 (14)	0.0219 (14)	0.0151 (14)
C22	0.090 (2)	0.0500 (18)	0.075 (2)	−0.0031 (15)	0.0045 (17)	0.0058 (15)
S2	0.0754 (5)	0.0472 (4)	0.0500 (4)	0.0045 (3)	0.0053 (4)	0.0072 (3)
O5	0.1063 (16)	0.1152 (17)	0.0936 (15)	0.0018 (14)	0.0490 (13)	0.0518 (14)
O6	0.1197 (17)	0.0801 (15)	0.0861 (14)	0.0241 (12)	0.0650 (13)	0.0012 (11)
O7	0.0705 (12)	0.0642 (12)	0.0706 (12)	0.0332 (9)	0.0346 (10)	0.0331 (9)
O8	0.0566 (11)	0.0493 (10)	0.0647 (11)	0.0089 (8)	0.0343 (9)	0.0110 (8)
N4	0.0476 (13)	0.0432 (12)	0.0520 (12)	0.0203 (9)	0.0248 (11)	0.0162 (10)
N5	0.0449 (13)	0.0441 (13)	0.0593 (13)	0.0053 (10)	0.0262 (11)	0.0050 (10)
N6	0.0571 (14)	0.0381 (13)	0.0690 (14)	0.0056 (10)	0.0339 (11)	0.0070 (10)
C23	0.0537 (17)	0.0614 (18)	0.0453 (15)	0.0084 (13)	0.0118 (13)	0.0187 (13)
C24	0.0579 (18)	0.085 (2)	0.0496 (17)	−0.0002 (16)	0.0153 (14)	0.0268 (16)
C25	0.0629 (19)	0.100 (2)	0.0521 (18)	0.0106 (17)	0.0323 (15)	0.0220 (17)
C26	0.0529 (18)	0.074 (2)	0.0525 (18)	0.0119 (15)	0.0166 (14)	0.0036 (16)
C27	0.0567 (17)	0.0595 (19)	0.0496 (16)	0.0050 (13)	0.0226 (14)	0.0068 (13)
C28	0.0393 (15)	0.0528 (17)	0.0417 (15)	0.0055 (12)	0.0124 (12)	0.0117 (13)
C29	0.131 (3)	0.091 (3)	0.103 (3)	−0.014 (2)	0.028 (2)	0.049 (2)
C30	0.187 (3)	0.121 (3)	0.125 (3)	0.059 (2)	0.116 (3)	0.011 (2)
C31	0.0425 (16)	0.0466 (17)	0.0475 (16)	0.0037 (12)	0.0138 (13)	0.0107 (13)
C32	0.0397 (16)	0.0284 (13)	0.0468 (15)	0.0076 (11)	0.0155 (13)	0.0079 (11)
C33	0.0343 (15)	0.0554 (16)	0.0507 (16)	0.0089 (11)	0.0116 (13)	0.0107 (12)
C34	0.0554 (18)	0.0485 (16)	0.0423 (15)	0.0078 (13)	0.0127 (14)	0.0116 (12)
C35	0.0438 (16)	0.0297 (14)	0.0507 (16)	0.0057 (11)	0.0186 (13)	0.0070 (11)

C36	0.0343 (15)	0.0469 (16)	0.0611 (17)	0.0100 (11)	0.0167 (14)	0.0144 (12)
C37	0.0424 (16)	0.0548 (16)	0.0483 (15)	0.0105 (12)	0.0111 (13)	0.0192 (12)
C38	0.0393 (15)	0.0389 (15)	0.0434 (15)	0.0061 (11)	0.0142 (12)	0.0085 (11)
C39	0.0476 (16)	0.0501 (17)	0.0545 (16)	0.0026 (12)	0.0240 (13)	0.0105 (13)
C40	0.0509 (17)	0.0596 (18)	0.0563 (17)	0.0062 (13)	0.0317 (14)	0.0023 (14)
C41	0.0337 (14)	0.0412 (15)	0.0450 (15)	0.0061 (11)	0.0140 (12)	0.0079 (12)
C42	0.0384 (14)	0.0412 (15)	0.0413 (14)	0.0093 (11)	0.0170 (11)	0.0064 (11)
C43	0.0436 (16)	0.0383 (16)	0.0470 (16)	0.0098 (12)	0.0116 (13)	0.0091 (12)
C44	0.082 (2)	0.0438 (17)	0.090 (2)	0.0045 (14)	0.0416 (17)	0.0110 (14)

Geometric parameters (Å, º)

S1—C35	1.7682 (19)	C22—H22C	0.9600
S1—C38	1.761 (2)	C22—H22A	0.9600
O1—C2	1.361 (2)	O5—C24	1.358 (2)
O1—C7	1.430 (2)	O5—C29	1.413 (3)
O2—C4	1.362 (2)	O6—C26	1.368 (3)
O2—C8	1.414 (2)	O6—C30	1.411 (2)
O3—C9	1.222 (2)	O7—C31	1.218 (2)
O4—C21	1.235 (2)	O8—C43	1.231 (2)
N1—H1	0.8600	N4—H4	0.8600
N1—C9	1.359 (2)	N4—C31	1.366 (2)
N1—C10	1.412 (2)	N4—C32	1.415 (2)
N2—C18	1.332 (3)	N5—C40	1.342 (2)
N2—C19	1.335 (2)	N5—C41	1.339 (2)
N3—H3	0.8600	N6—H6	0.8600
N3—C21	1.328 (2)	N6—C43	1.317 (2)
N3—C22	1.458 (2)	N6—C44	1.451 (2)
C1—H1A	0.9300	C23—H23	0.9300
C1—C2	1.387 (3)	C23—C24	1.387 (3)
C1—C6	1.378 (2)	C23—C28	1.396 (2)
C2—C3	1.375 (3)	C24—C25	1.394 (3)
C3—H3A	0.9300	C25—H25	0.9300
C3—C4	1.392 (3)	C25—C26	1.365 (3)
C4—C5	1.380 (3)	C26—C27	1.390 (3)
C5—H5	0.9300	C27—H27	0.9300
C5—C6	1.395 (3)	C27—C28	1.365 (2)
C6—C9	1.498 (3)	C28—C31	1.491 (3)
C7—H7B	0.9600	C29—H29A	0.9600
C7—H7C	0.9600	C29—H29B	0.9600
C7—H7A	0.9600	C29—H29C	0.9600
C8—H8C	0.9600	C30—H30A	0.9600
C8—H8B	0.9600	C30—H30B	0.9600
C8—H8A	0.9600	C30—H30C	0.9600
C10—C11	1.386 (3)	C32—C33	1.377 (2)
C10—C15	1.380 (2)	C32—C37	1.376 (2)
C11—H11	0.9300	C33—H33	0.9300
C11—C12	1.371 (3)	C33—C34	1.383 (2)

C12—H12	0.9300	C34—H34	0.9300
C12—C13	1.391 (2)	C34—C35	1.381 (2)
C13—C14	1.378 (3)	C35—C36	1.383 (3)
C13—S2	1.768 (2)	C36—H36	0.9300
C14—H14	0.9300	C36—C37	1.384 (2)
C14—C15	1.383 (3)	C37—H37	0.9300
C15—H15	0.9300	C38—C39	1.385 (2)
C16—C17	1.382 (3)	C38—C42	1.376 (2)
C16—C20	1.381 (3)	C39—H39	0.9300
C16—S2	1.757 (2)	C39—C40	1.369 (2)
C17—H17	0.9300	C40—H40	0.9300
C17—C18	1.380 (3)	C41—C42	1.378 (2)
C18—H18	0.9300	C41—C43	1.509 (3)
C19—C20	1.388 (2)	C42—H42	0.9300
C19—C21	1.507 (3)	C44—H44B	0.9600
C20—H20	0.9300	C44—H44C	0.9600
C22—H22B	0.9600	C44—H44A	0.9600

O1—C2—C1	115.0 (2)	O5—C24—C23	124.4 (3)
O1—C2—C3	124.5 (2)	O5—C24—C25	115.1 (2)
O1—C7—H7B	109.5	O5—C29—H29A	109.5
O1—C7—H7C	109.5	O5—C29—H29B	109.5
O1—C7—H7A	109.5	O5—C29—H29C	109.5
O2—C4—C3	114.4 (2)	O6—C26—C27	114.7 (2)
O2—C4—C5	124.6 (2)	O6—C30—H30A	109.5
O2—C8—H8C	109.5	O6—C30—H30B	109.5
O2—C8—H8B	109.5	O6—C30—H30C	109.5
O2—C8—H8A	109.5	O7—C31—N4	122.79 (19)
O3—C9—N1	123.0 (2)	O7—C31—C28	122.51 (19)
O3—C9—C6	122.3 (2)	O8—C43—N6	124.05 (19)
O4—C21—N3	123.5 (2)	O8—C43—C41	120.4 (2)
O4—C21—C19	121.2 (2)	N4—C31—C28	114.70 (19)
N1—C9—C6	114.6 (2)	N5—C40—C39	125.08 (19)
N2—C18—C17	124.9 (2)	N5—C40—H40	117.5
N2—C18—H18	117.5	N5—C41—C42	123.90 (18)
N2—C19—C20	124.2 (2)	N5—C41—C43	117.27 (19)
N2—C19—C21	117.5 (2)	N6—C43—C41	115.56 (19)
N3—C21—C19	115.3 (2)	N6—C44—H44B	109.5
N3—C22—H22B	109.5	N6—C44—H44C	109.5
N3—C22—H22C	109.5	N6—C44—H44A	109.5
N3—C22—H22A	109.5	C23—C24—C25	120.5 (2)
C1—C6—C5	120.9 (2)	C23—C28—C31	118.6 (2)
C1—C6—C9	121.8 (2)	C24—O5—C29	118.1 (2)
C2—O1—C7	116.82 (17)	C24—C23—H23	121.0
C2—C1—H1A	120.2	C24—C23—C28	118.1 (2)
C2—C3—H3A	120.3	C24—C25—H25	119.9
C2—C3—C4	119.4 (2)	C25—C26—O6	125.5 (2)
C3—C2—C1	120.5 (2)	C25—C26—C27	119.8 (2)

C4—O2—C8	118.42 (19)	C26—O6—C30	117.80 (19)
C4—C3—H3A	120.3	C26—C25—C24	120.3 (2)
C4—C5—H5	120.7	C26—C25—H25	119.9
C4—C5—C6	118.6 (2)	C26—C27—H27	120.0
C5—C4—C3	121.0 (2)	C27—C28—C23	121.31 (19)
C5—C6—C9	117.3 (2)	C27—C28—C31	120.11 (19)
C6—C1—H1A	120.2	C28—C23—H23	121.0
C6—C1—C2	119.6 (2)	C28—C27—C26	120.0 (2)
C6—C5—H5	120.7	C28—C27—H27	120.0
H7B—C7—H7C	109.5	H29A—C29—H29B	109.5
H7B—C7—H7A	109.5	H29A—C29—H29C	109.5
H7C—C7—H7A	109.5	H29B—C29—H29C	109.5
H8C—C8—H8B	109.5	H30A—C30—H30B	109.5
H8C—C8—H8A	109.5	H30A—C30—H30C	109.5
H8B—C8—H8A	109.5	H30B—C30—H30C	109.5
C9—N1—H1	117.5	C31—N4—H4	118.2
C9—N1—C10	125.04 (19)	C31—N4—C32	123.61 (17)
C10—N1—H1	117.5	C32—N4—H4	118.2
C10—C11—H11	119.9	C32—C33—H33	119.7
C10—C15—C14	120.7 (2)	C32—C33—C34	120.7 (2)
C10—C15—H15	119.7	C32—C37—C36	120.4 (2)
C11—C10—N1	121.4 (2)	C32—C37—H37	119.8
C11—C12—H12	119.5	C33—C32—N4	119.8 (2)
C11—C12—C13	120.9 (2)	C33—C34—H34	119.8
C12—C11—C10	120.2 (2)	C34—C33—H33	119.7
C12—C11—H11	119.9	C34—C35—S1	121.10 (18)
C12—C13—S2	119.56 (18)	C34—C35—C36	118.69 (19)
C13—C12—H12	119.5	C35—C34—C33	120.5 (2)
C13—C14—H14	119.8	C35—C34—H34	119.8
C13—C14—C15	120.4 (2)	C35—C36—H36	119.7
C14—C13—C12	118.7 (2)	C35—C36—C37	120.6 (2)
C14—C13—S2	121.66 (18)	C36—C35—S1	120.15 (17)
C14—C15—H15	119.7	C36—C37—H37	119.8
C15—C10—N1	119.5 (2)	C37—C32—N4	121.0 (2)
C15—C10—C11	119.0 (2)	C37—C32—C33	119.08 (19)
C15—C14—H14	119.8	C37—C36—H36	119.7
C16—C17—H17	120.6	C38—S1—C35	103.42 (9)
C16—C20—C19	119.1 (2)	C38—C39—H39	120.6
C16—C20—H20	120.5	C38—C42—C41	119.88 (17)
C16—S2—C13	102.47 (10)	C38—C42—H42	120.1
C17—C16—S2	118.17 (19)	C39—C38—S1	118.50 (15)
C17—C18—H18	117.5	C39—C40—H40	117.5
C18—N2—C19	115.4 (2)	C40—C39—C38	118.88 (18)
C18—C17—C16	118.8 (2)	C40—C39—H39	120.6
C18—C17—H17	120.6	C41—N5—C40	115.00 (18)
C19—C20—H20	120.5	C41—C42—H42	120.1
C20—C16—C17	117.5 (2)	C42—C38—S1	124.27 (15)
C20—C16—S2	124.28 (18)	C42—C38—C39	117.22 (19)

C20—C19—C21	118.4 (2)	C42—C41—C43	118.77 (18)
C21—N3—H3	118.9	C43—N6—H6	118.7
C21—N3—C22	122.1 (2)	C43—N6—C44	122.66 (17)
C22—N3—H3	118.9	C44—N6—H6	118.7
H22B—C22—H22C	109.5	H44B—C44—H44C	109.5
H22B—C22—H22A	109.5	H44B—C44—H44A	109.5
H22C—C22—H22A	109.5	H44C—C44—H44A	109.5
S1—C35—C36—C37	−177.77 (14)	S2—C13—C14—C15	178.39 (16)
S1—C38—C39—C40	179.83 (17)	S2—C16—C17—C18	178.32 (16)
S1—C38—C42—C41	−179.13 (15)	S2—C16—C20—C19	−177.09 (14)
O1—C2—C3—C4	179.82 (17)	O5—C24—C25—C26	179.0 (2)
O2—C4—C5—C6	−178.31 (19)	O6—C26—C27—C28	−179.1 (2)
N1—C10—C11—C12	179.40 (19)	N4—C32—C33—C34	−179.35 (17)
N1—C10—C15—C14	−179.2 (2)	N4—C32—C37—C36	179.74 (17)
N2—C19—C20—C16	−2.2 (3)	N5—C41—C42—C38	−1.4 (3)
N2—C19—C21—O4	−177.59 (19)	N5—C41—C43—O8	174.55 (19)
N2—C19—C21—N3	3.5 (3)	N5—C41—C43—N6	−5.3 (3)
C1—C2—C3—C4	−1.8 (3)	C23—C24—C25—C26	−0.8 (4)
C1—C6—C9—O3	−149.3 (2)	C23—C28—C31—O7	34.5 (3)
C1—C6—C9—N1	32.3 (3)	C23—C28—C31—N4	−144.92 (19)
C2—C1—C6—C5	2.1 (3)	C24—C23—C28—C27	−2.4 (3)
C2—C1—C6—C9	−176.02 (18)	C24—C23—C28—C31	179.0 (2)
C2—C3—C4—O2	−179.76 (18)	C24—C25—C26—O6	179.3 (2)
C2—C3—C4—C5	2.2 (3)	C24—C25—C26—C27	−1.1 (4)
C3—C4—C5—C6	−0.5 (3)	C25—C26—C27—C28	1.3 (3)
C4—C5—C6—C1	−1.7 (3)	C26—C27—C28—C23	0.5 (3)
C4—C5—C6—C9	176.49 (19)	C26—C27—C28—C31	179.1 (2)
C5—C6—C9—O3	32.5 (3)	C27—C28—C31—O7	−144.2 (2)
C5—C6—C9—N1	−145.87 (19)	C27—C28—C31—N4	36.4 (3)
C6—C1—C2—O1	178.23 (15)	C28—C23—C24—O5	−177.3 (2)
C6—C1—C2—C3	−0.3 (3)	C28—C23—C24—C25	2.5 (3)
C7—O1—C2—C1	−177.90 (17)	C29—O5—C24—C23	0.6 (4)
C7—O1—C2—C3	0.6 (3)	C29—O5—C24—C25	−179.1 (2)
C8—O2—C4—C3	177.17 (18)	C30—O6—C26—C25	2.2 (4)
C8—O2—C4—C5	−4.8 (3)	C30—O6—C26—C27	−177.3 (2)
C9—N1—C10—C11	36.4 (3)	C31—N4—C32—C33	−139.0 (2)
C9—N1—C10—C15	−145.8 (2)	C31—N4—C32—C37	44.2 (3)
C10—N1—C9—O3	4.0 (4)	C32—N4—C31—O7	5.9 (3)
C10—N1—C9—C6	−177.61 (19)	C32—N4—C31—C28	−174.73 (18)
C10—C11—C12—C13	−0.7 (3)	C32—C33—C34—C35	0.5 (3)
C11—C10—C15—C14	−1.3 (3)	C33—C32—C37—C36	2.9 (3)
C11—C12—C13—C14	−0.6 (3)	C33—C34—C35—S1	178.18 (15)
C11—C12—C13—S2	−178.15 (16)	C33—C34—C35—C36	1.1 (3)
C12—C13—C14—C15	0.9 (3)	C34—C35—C36—C37	−0.7 (3)
C12—C13—S2—C16	−68.06 (18)	C35—S1—C38—C39	175.66 (17)
C13—C14—C15—C10	0.1 (3)	C35—S1—C38—C42	−5.7 (2)
C14—C13—S2—C16	114.47 (18)	C35—C36—C37—C32	−1.4 (3)

C15—C10—C11—C12	1.6 (3)	C37—C32—C33—C34	−2.5 (3)
C16—C17—C18—N2	−0.3 (4)	C38—S1—C35—C34	96.53 (17)
C17—C16—C20—C19	1.8 (3)	C38—S1—C35—C36	−86.45 (18)
C17—C16—S2—C13	161.70 (16)	C38—C39—C40—N5	0.1 (3)
C18—N2—C19—C20	1.3 (3)	C39—C38—C42—C41	−0.5 (3)
C18—N2—C19—C21	−177.12 (18)	C40—N5—C41—C42	2.5 (3)
C19—N2—C18—C17	0.0 (3)	C40—N5—C41—C43	−174.82 (18)
C20—C16—C17—C18	−0.6 (3)	C41—N5—C40—C39	−1.8 (3)
C20—C16—S2—C13	−19.4 (2)	C42—C38—C39—C40	1.1 (3)
C20—C19—C21—O4	3.9 (3)	C42—C41—C43—O8	−2.9 (3)
C20—C19—C21—N3	−174.95 (17)	C42—C41—C43—N6	177.22 (19)
C21—C19—C20—C16	176.16 (17)	C43—C41—C42—C38	175.86 (17)
C22—N3—C21—O4	−3.2 (3)	C44—N6—C43—O8	−3.8 (3)
C22—N3—C21—C19	175.66 (17)	C44—N6—C43—C41	176.07 (17)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O4^{i}	0.86	2.12	2.941 (2)	159
N3—H3···O7^{ii}	0.86	2.22	2.922 (2)	138
N4—H4···O8^{iii}	0.86	2.15	2.985 (2)	163
N6—H6···O3^{iv}	0.86	2.30	2.957 (2)	133

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