Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Methyl 3-[(6-nitro-4-oxo-3-phenyl-3,4-dihydroquinazolin-2-yl)sulfanyl]propanoate

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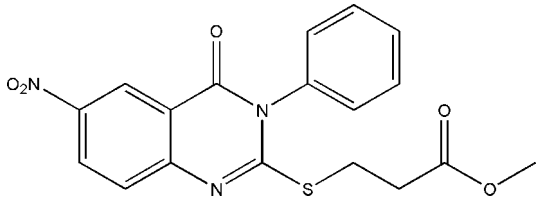
Received 29 May 2013; accepted 10 June 2013

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.007 Å; disorder in main residue; R factor = 0.064; wR factor = 0.191; data-to-parameter ratio = 12.4.

In the title compound, $C_{18}H_{15}N_3O_5S$, the approximately planar quinazoline ring system [maximum deviation = 0.097 (3) Å] forms a dihedral angle of 76.53 (19)° with the phenyl ring. The terminal -C(=O)—O—C group is disordered over two sets of sites with a site-occupancy ratio of 0.811 (17):0.189 (17). In the crystal, molecules are linked *via* weak C—H···O hydrogen bonds into sheets parallel to the *ac* plane.

Related literature

For background to quinazoline chemistry, see: El-Azab (2007); El-Azab *et al.* (2010, 2011); Alafeefy *et al.* (2008); Al-Suwaidan *et al.* (2013); El-Azab & ElTahir (2012*a*,*b*). For standard bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{18}H_{15}N_3O_5S$ M_r = 385.39
Monoclinic, $P2_1/n$
a = 4.9146 (3) Å
b = 26.5065 (18) Å
c = 14.0900 (9) Å
β = 94.645 (4)°
V = 1829.5 (2) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 1.89 mm^{-1}
T = 296 K
0.32 × 0.26 × 0.13 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.583, T_{max} = 0.791
12669 measured reflections
3382 independent reflections
1861 reflections with $I > 2\sigma(I)$
R_{int} = 0.059

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.191
S = 1.03
3382 reflections
273 parameters
9 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6A···O2^{i}	0.93	2.56	3.142 (5)	121
C10—H10A···O2^{ii}	0.93	2.39	3.167 (5)	140

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

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

The authors thank the Deanship of Scientific Research and the Research Center of the College of Pharmacy, King Saud University. CSC thanks Universiti Sains Malaysia for a post-doctoral research fellowship.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5622).

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‡ Thomson Reuters ResearcherID: C-3194-2011.
§ Thomson Reuters ResearcherID: A-3561-2009.

supplementary materials

Acta Cryst. (2013). E**69**, o1111 [doi:10.1107/S1600536813016127]

Methyl 3-[(6-nitro-4-oxo-3-phenyl-3,4-dihydroquinazolin-2-yl)sulfanyl]propanoate

Ibrahim A. Al-Suwaidan, Alaa A.-M. Abdel-Aziz, Adel S. El-Azab, C. S. Chidan Kumar and Hoong-Kun Fun

Comment

Quinazolines are considered to be important chemical synthons of physiological significance and pharmaceutical utility. They possess a variety of biological effects including antimicrobial (El-Azab *et al.*, 2007), anti-inflammatory (Alafeefy *et al.*, 2008), anticonvulsant, (El-Azab *et al.*, 2011; El-Azab & ElTahir 2012*a*,*b*) and anticancer activities (El-Azab *et al.*, 2010; El-Azab & ElTahir 2012*b*; Al-Suwaidan *et al.*, 2013). These observations have been the guidelines for the development of new quinazolines which possess varied biological activities. Prompted by the potential biological activities of quinazolines, the title compound was synthesized and its crystal structure is reported herein.

The molecular structure of the title compound is shown in Fig. 1. The quinazoline ring (C1–C8/N1–N2; maximum deviation = 0.097 (3) Å at atom N2) makes a dihedral angle of 76.53 (19)° with the attached phenyl ring (C9–C14). The terminal C17(═O1)—O5—C18 group is disordered over two positions with a site-occupancy ratio of 0.811 (17): 0.189 (17). In the crystal structure (Fig. 2), the molecules are linked *via* weak intermolecular C6—H6A···O2^{i} and C10—H10A···O2^{ii} hydrogen bonds (see Table 1 for symmetry codes) into sheets parallel to the *ac* plane.

Experimental

A mixture of 3-phenyl-2-mercapto-6-nitro-quinazolin-4(3*H*)-one (2.99 g, 0.01 mol) and Et_3N (2 ml) in CH_2Cl_2 (30 ml) was stirred in an ice bath and acryloyl chloride (3.3 ml, 0.04 mol) was added dropwise over a period of 15 min. Stirring was performed in an ice bath for 1 h and then at room temperature overnight. Solvent was then removed under reduced pressure and the obtained residue was dissolved in CH_2Cl_2 and washed with 10% NaOH solution and water. The resultant was separated and dried over $MgSO_4$ then evaporated *in vacuo*. The obtained residue was chromatographed on silica gel using 10% EtOAc/hexane as eluant and recrystallized from hexane/CH_2Cl_2 (92%) (m.p:. 480 K) to yield X-ray quality crystals.

Refinement

The hydrogen atoms were positioned geometrically [C–H = 0.93, 0.96 and 0.97 Å] and were refined using a riding model, with U_{iso}(H) = 1.2 U_{eq}(C) or 1.5U_{eq}(methyl C). A rotating-group model was used for the methyl groups. The terminal C17(═O1)—O5—C18 group is disordered over two positions with a site-occupancy ratio of 0.811 (17): 0.189 (17). The SHELXL (Sheldrick, 2008) EXYZ (same *x*, *y* and *z* parameters) and EADP (same U_{ij} parameters) restraints were used for atoms pairs C17/C17A.The same distance restraints were applied to (C17/O1 & C17A/O1A), (C17/O5 & C17A/O5A) and (C18/O5 & C18A/O5A). The SIMU (similar U_{ij} parameters) restraint was applied to C18/C18A.

Computing details

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

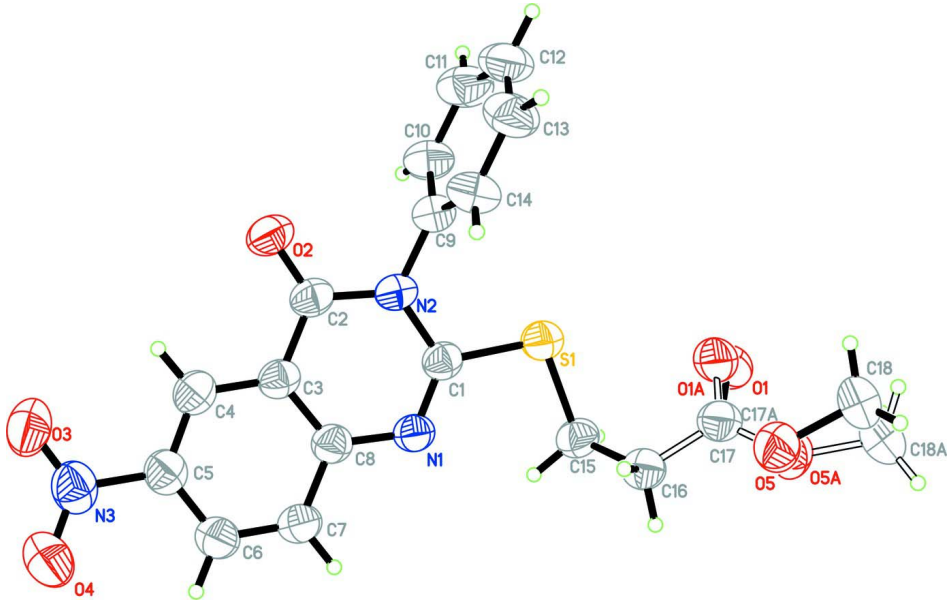

Figure 1

The molecular structure of the title compound with 30% probability displacement ellipsoids. The minor component of disorder is shown as open bonds

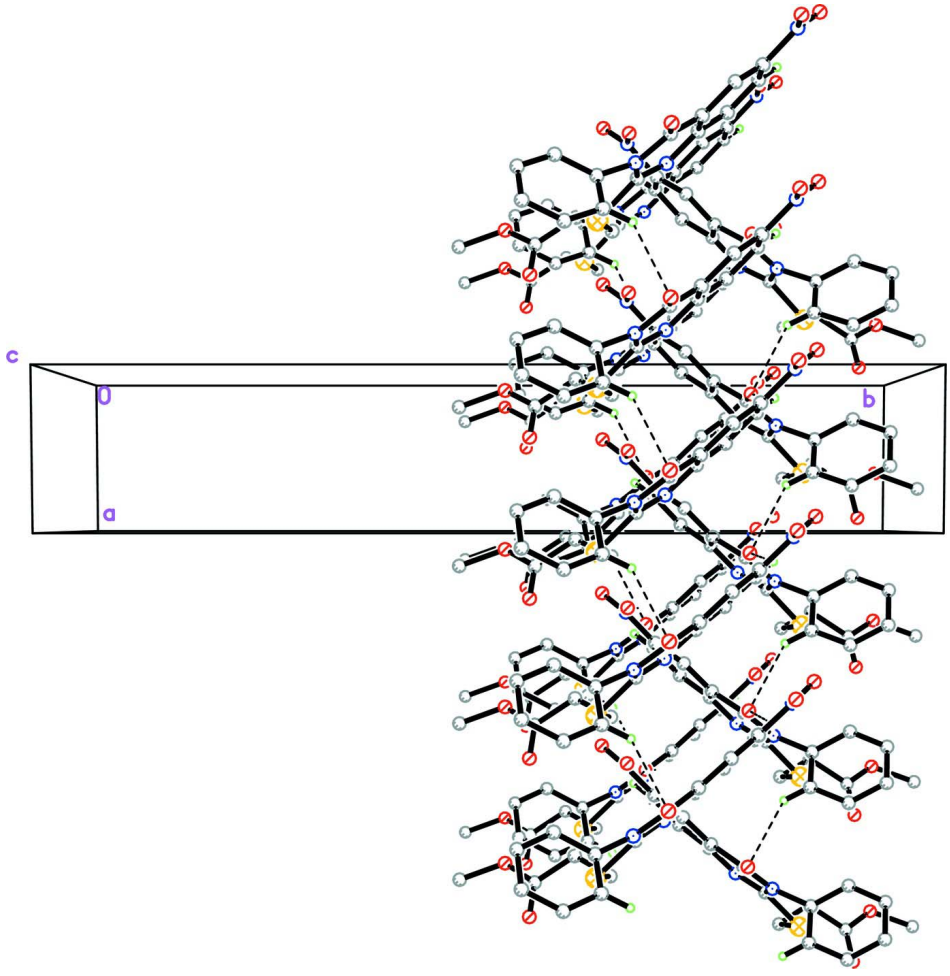

Figure 2

The crystal packing of the title compound. The minor component of disorder and H atoms not involved in the intermolecular interactions (dashed lines) have been omitted for clarity.

Methyl 3-[(6-nitro-4-oxo-3-phenyl-3,4-dihydroquinazolin-2-yl)sulfanyl]propanoate

Crystal data

$C_{18}H_{15}N_3O_5S$
$M_r = 385.39$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 4.9146\ (3)$ Å
$b = 26.5065\ (18)$ Å
$c = 14.0900\ (9)$ Å
$\beta = 94.645\ (4)°$
$V = 1829.5\ (2)$ Å^3
$Z = 4$

$F(000) = 800$
$D_x = 1.399$ Mg m^{-3}
Melting point: 480 K
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 1209 reflections
$\theta = 3.3–67.5°$
$\mu = 1.89$ mm^{-1}
$T = 296$ K
Block, colourless
0.32 × 0.26 × 0.13 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.583, T_{max} = 0.791
12669 measured reflections
3382 independent reflections
1861 reflections with $I > 2\sigma(I)$
R_{int} = 0.059
θ_{max} = 69.8°, θ_{min} = 3.3°
$h = -5 \rightarrow 4$
$k = -31 \rightarrow 31$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.191
S = 1.03
3382 reflections
273 parameters
9 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
$w = 1/[\sigma^2(F_o^2) + (0.0825P)^2 + 0.1932P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Extinction correction: *SHELXTL* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0030 (5)

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.

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
S1	0.3830 (2)	0.12146 (4)	0.63782 (7)	0.0880 (4)	
O2	0.8688 (6)	0.19581 (12)	0.38141 (18)	0.0982 (9)	
O3	1.5168 (8)	0.33688 (17)	0.4490 (3)	0.1442 (16)	
O4	1.6007 (9)	0.36422 (17)	0.5910 (3)	0.1520 (16)	
N1	0.7309 (6)	0.19860 (13)	0.6615 (2)	0.0790 (9)	
N2	0.6827 (6)	0.16072 (12)	0.50857 (19)	0.0741 (8)	
N3	1.4799 (8)	0.33704 (17)	0.5326 (4)	0.1094 (13)	
C1	0.6245 (7)	0.16499 (15)	0.6034 (2)	0.0738 (9)	
C2	0.8395 (7)	0.19721 (16)	0.4673 (3)	0.0786 (10)	
C3	0.9676 (7)	0.23374 (15)	0.5321 (2)	0.0760 (10)	
C4	1.1534 (8)	0.26847 (16)	0.5010 (3)	0.0849 (11)	
H4A	1.1912	0.2694	0.4374	0.102*	
C5	1.2796 (8)	0.30119 (17)	0.5656 (3)	0.0884 (11)	
C6	1.2314 (9)	0.30066 (18)	0.6598 (3)	0.0984 (13)	
H6A	1.3229	0.3229	0.7023	0.118*	

C7	1.0479 (9)	0.26718 (17)	0.6906 (3)	0.0927 (12)	
H7A	1.0117	0.2671	0.7544	0.111*	
C8	0.9117 (7)	0.23265 (15)	0.6269 (3)	0.0787 (10)	
C9	0.5906 (7)	0.11756 (17)	0.4514 (2)	0.0783 (10)	
C10	0.3811 (8)	0.1233 (2)	0.3819 (3)	0.0991 (14)	
H10A	0.2985	0.1545	0.3706	0.119*	
C11	0.2955 (11)	0.0814 (3)	0.3288 (4)	0.1243 (19)	
H11A	0.1516	0.0844	0.2820	0.149*	
C12	0.4181 (12)	0.0363 (3)	0.3440 (4)	0.1245 (19)	
H12A	0.3567	0.0084	0.3085	0.149*	
C13	0.6334 (11)	0.0314 (2)	0.4119 (4)	0.1198 (17)	
H13A	0.7208	0.0004	0.4212	0.144*	
C14	0.7186 (9)	0.07209 (18)	0.4656 (3)	0.1008 (14)	
H14A	0.8636	0.0689	0.5118	0.121*	
C15	0.3526 (9)	0.14022 (17)	0.7595 (2)	0.0889 (12)	
H15A	0.4555	0.1710	0.7724	0.107*	
H15B	0.1625	0.1473	0.7682	0.107*	
C16	0.4560 (8)	0.09993 (17)	0.8302 (3)	0.0871 (11)	
H16A	0.6427	0.0916	0.8188	0.105*	
H16B	0.4572	0.1136	0.8941	0.105*	
C17	0.2895 (9)	0.05291 (19)	0.8246 (3)	0.0925 (13)	0.811 (17)
O1	0.085 (3)	0.0464 (8)	0.7732 (11)	0.107 (4)	0.811 (17)
O5	0.4116 (19)	0.0176 (3)	0.8814 (6)	0.118 (3)	0.811 (17)
C18	0.264 (3)	−0.0316 (3)	0.8826 (7)	0.157 (4)	0.811 (17)
H18A	0.3690	−0.0551	0.9223	0.235*	0.811 (17)
H18B	0.2381	−0.0447	0.8190	0.235*	0.811 (17)
H18C	0.0892	−0.0266	0.9072	0.235*	0.811 (17)
C17A	0.2895 (9)	0.05291 (19)	0.8246 (3)	0.0925 (13)	0.189 (17)
O1A	0.120 (14)	0.048 (4)	0.759 (5)	0.115 (18)	0.189 (17)
O5A	0.293 (6)	0.0223 (10)	0.9005 (15)	0.089 (7)	0.189 (17)
C18A	0.134 (10)	−0.0214 (14)	0.934 (3)	0.156 (7)	0.189 (17)
H18D	0.2131	−0.0324	0.9952	0.234*	0.189 (17)
H18E	0.1376	−0.0486	0.8893	0.234*	0.189 (17)
H18F	−0.0517	−0.0112	0.9396	0.234*	0.189 (17)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0921 (7)	0.0934 (8)	0.0790 (6)	−0.0061 (5)	0.0095 (4)	−0.0080 (6)
O2	0.119 (2)	0.109 (3)	0.0674 (15)	0.0031 (17)	0.0072 (13)	−0.0014 (16)
O3	0.148 (3)	0.169 (4)	0.119 (3)	−0.039 (3)	0.023 (2)	0.034 (3)
O4	0.163 (4)	0.138 (4)	0.153 (3)	−0.056 (3)	−0.003 (3)	0.003 (3)
N1	0.092 (2)	0.077 (2)	0.0678 (17)	0.0000 (16)	0.0039 (14)	−0.0049 (17)
N2	0.0814 (19)	0.078 (2)	0.0622 (16)	0.0074 (15)	0.0006 (13)	−0.0056 (16)
N3	0.103 (3)	0.103 (3)	0.120 (3)	−0.006 (2)	−0.004 (2)	0.024 (3)
C1	0.080 (2)	0.073 (3)	0.068 (2)	0.0073 (17)	0.0035 (15)	0.001 (2)
C2	0.086 (2)	0.083 (3)	0.066 (2)	0.012 (2)	−0.0007 (17)	0.001 (2)
C3	0.088 (2)	0.071 (3)	0.068 (2)	0.0111 (19)	0.0005 (16)	0.0045 (19)
C4	0.090 (3)	0.085 (3)	0.079 (2)	0.010 (2)	0.0033 (19)	0.013 (2)

C5	0.092 (3)	0.080 (3)	0.092 (3)	0.002 (2)	−0.002 (2)	0.012 (2)
C6	0.117 (3)	0.089 (3)	0.088 (3)	−0.016 (3)	−0.006 (2)	0.001 (3)
C7	0.116 (3)	0.091 (3)	0.071 (2)	−0.007 (2)	0.003 (2)	−0.004 (2)
C8	0.090 (2)	0.072 (3)	0.073 (2)	0.0019 (19)	0.0002 (17)	0.001 (2)
C9	0.082 (2)	0.086 (3)	0.067 (2)	0.004 (2)	0.0031 (16)	−0.007 (2)
C10	0.095 (3)	0.115 (4)	0.085 (3)	0.009 (2)	−0.010 (2)	−0.016 (3)
C11	0.111 (4)	0.161 (6)	0.098 (3)	−0.008 (4)	−0.015 (3)	−0.030 (4)
C12	0.129 (4)	0.137 (6)	0.108 (4)	−0.031 (4)	0.012 (3)	−0.049 (4)
C13	0.136 (4)	0.095 (4)	0.130 (4)	0.000 (3)	0.016 (3)	−0.038 (3)
C14	0.104 (3)	0.095 (4)	0.100 (3)	0.006 (3)	−0.008 (2)	−0.026 (3)
C15	0.100 (3)	0.093 (3)	0.076 (2)	0.003 (2)	0.0171 (19)	−0.008 (2)
C16	0.082 (2)	0.094 (3)	0.085 (2)	−0.001 (2)	0.0058 (19)	−0.007 (2)
C17	0.092 (3)	0.102 (4)	0.083 (3)	−0.011 (2)	0.005 (2)	−0.009 (3)
O1	0.089 (5)	0.119 (7)	0.110 (6)	−0.015 (5)	−0.006 (6)	−0.006 (5)
O5	0.132 (6)	0.111 (4)	0.109 (4)	−0.017 (4)	−0.014 (4)	0.020 (3)
C18	0.229 (11)	0.110 (6)	0.130 (7)	−0.069 (7)	0.011 (6)	0.006 (5)
C17A	0.092 (3)	0.102 (4)	0.083 (3)	−0.011 (2)	0.005 (2)	−0.009 (3)
O1A	0.10 (3)	0.14 (3)	0.10 (2)	−0.05 (2)	0.028 (16)	−0.02 (2)
O5A	0.083 (15)	0.101 (15)	0.082 (12)	−0.005 (11)	−0.005 (9)	0.027 (10)
C18A	0.226 (15)	0.103 (11)	0.137 (12)	−0.061 (11)	0.004 (11)	−0.006 (11)

Geometric parameters (Å, º)

S1—C1	1.752 (4)	C10—H10A	0.9300
S1—C15	1.803 (4)	C11—C12	1.348 (7)
O2—C2	1.231 (4)	C11—H11A	0.9300
O3—N3	1.207 (5)	C12—C13	1.374 (7)
O4—N3	1.212 (5)	C12—H12A	0.9300
N1—C1	1.291 (4)	C13—C14	1.364 (6)
N1—C8	1.382 (5)	C13—H13A	0.9300
N2—C2	1.393 (5)	C14—H14A	0.9300
N2—C1	1.394 (4)	C15—C16	1.519 (5)
N2—C9	1.451 (5)	C15—H15A	0.9700
N3—C5	1.470 (6)	C15—H15B	0.9700
C2—C3	1.440 (5)	C16—C17	1.489 (6)
C3—C8	1.386 (5)	C16—H16A	0.9700
C3—C4	1.393 (5)	C16—H16B	0.9700
C4—C5	1.369 (5)	C17—O1	1.204 (7)
C4—H4A	0.9300	C17—O5	1.342 (6)
C5—C6	1.367 (6)	O5—C18	1.494 (8)
C6—C7	1.361 (6)	C18—H18A	0.9600
C6—H6A	0.9300	C18—H18B	0.9600
C7—C8	1.412 (5)	C18—H18C	0.9600
C7—H7A	0.9300	O5A—C18A	1.496 (9)
C9—C14	1.367 (6)	C18A—H18D	0.9600
C9—C10	1.371 (5)	C18A—H18E	0.9600
C10—C11	1.385 (7)	C18A—H18F	0.9600
C1—S1—C15	101.0 (2)	C12—C11—H11A	119.6
C1—N1—C8	117.8 (3)	C10—C11—H11A	119.6

C2—N2—C1	120.5 (3)	C11—C12—C13	120.3 (5)
C2—N2—C9	118.3 (3)	C11—C12—H12A	119.9
C1—N2—C9	121.2 (3)	C13—C12—H12A	119.9
O3—N3—O4	124.1 (5)	C14—C13—C12	119.7 (5)
O3—N3—C5	117.6 (5)	C14—C13—H13A	120.1
O4—N3—C5	118.3 (5)	C12—C13—H13A	120.1
N1—C1—N2	124.0 (4)	C13—C14—C9	120.0 (4)
N1—C1—S1	121.9 (3)	C13—C14—H14A	120.0
N2—C1—S1	114.1 (3)	C9—C14—H14A	120.0
O2—C2—N2	120.1 (4)	C16—C15—S1	112.3 (3)
O2—C2—C3	124.3 (4)	C16—C15—H15A	109.1
N2—C2—C3	115.5 (3)	S1—C15—H15A	109.1
C8—C3—C4	120.3 (4)	C16—C15—H15B	109.1
C8—C3—C2	119.1 (4)	S1—C15—H15B	109.1
C4—C3—C2	120.6 (3)	H15A—C15—H15B	107.9
C5—C4—C3	118.9 (4)	C17—C16—C15	113.6 (4)
C5—C4—H4A	120.6	C17—C16—H16A	108.8
C3—C4—H4A	120.6	C15—C16—H16A	108.8
C6—C5—C4	122.3 (4)	C17—C16—H16B	108.8
C6—C5—N3	119.1 (4)	C15—C16—H16B	108.8
C4—C5—N3	118.6 (4)	H16A—C16—H16B	107.7
C7—C6—C5	119.2 (4)	O1—C17—O5	124.8 (11)
C7—C6—H6A	120.4	O1—C17—C16	125.5 (11)
C5—C6—H6A	120.4	O5—C17—C16	109.6 (5)
C6—C7—C8	120.8 (4)	C17—O5—C18	114.9 (7)
C6—C7—H7A	119.6	O5—C18—H18A	109.5
C8—C7—H7A	119.6	O5—C18—H18B	109.5
N1—C8—C3	122.4 (3)	H18A—C18—H18B	109.5
N1—C8—C7	119.0 (3)	O5—C18—H18C	109.5
C3—C8—C7	118.6 (4)	H18A—C18—H18C	109.5
C14—C9—C10	120.8 (4)	H18B—C18—H18C	109.5
C14—C9—N2	119.7 (3)	O5A—C18A—H18D	109.5
C10—C9—N2	119.5 (4)	O5A—C18A—H18E	109.5
C9—C10—C11	118.4 (5)	H18D—C18A—H18E	109.5
C9—C10—H10A	120.8	O5A—C18A—H18F	109.5
C11—C10—H10A	120.8	H18D—C18A—H18F	109.5
C12—C11—C10	120.8 (5)	H18E—C18A—H18F	109.5

C8—N1—C1—N2	0.6 (5)	C1—N1—C8—C3	4.1 (6)
C8—N1—C1—S1	−177.5 (3)	C1—N1—C8—C7	−174.9 (3)
C2—N2—C1—N1	−7.6 (5)	C4—C3—C8—N1	−179.4 (3)
C9—N2—C1—N1	170.2 (3)	C2—C3—C8—N1	−1.9 (6)
C2—N2—C1—S1	170.6 (3)	C4—C3—C8—C7	−0.3 (6)
C9—N2—C1—S1	−11.6 (4)	C2—C3—C8—C7	177.2 (3)
C15—S1—C1—N1	0.6 (4)	C6—C7—C8—N1	178.7 (4)
C15—S1—C1—N2	−177.6 (3)	C6—C7—C8—C3	−0.4 (6)
C1—N2—C2—O2	−173.2 (3)	C2—N2—C9—C14	103.2 (4)
C9—N2—C2—O2	9.0 (5)	C1—N2—C9—C14	−74.6 (5)
C1—N2—C2—C3	9.3 (5)	C2—N2—C9—C10	−74.9 (5)

C9—N2—C2—C3	−168.6 (3)	C1—N2—C9—C10	107.2 (4)
O2—C2—C3—C8	177.8 (4)	C14—C9—C10—C11	2.4 (7)
N2—C2—C3—C8	−4.8 (5)	N2—C9—C10—C11	−179.5 (4)
O2—C2—C3—C4	−4.7 (6)	C9—C10—C11—C12	−1.0 (8)
N2—C2—C3—C4	172.7 (3)	C10—C11—C12—C13	−1.0 (9)
C8—C3—C4—C5	0.2 (6)	C11—C12—C13—C14	1.7 (8)
C2—C3—C4—C5	−177.3 (3)	C12—C13—C14—C9	−0.3 (8)
C3—C4—C5—C6	0.6 (6)	C10—C9—C14—C13	−1.7 (7)
C3—C4—C5—N3	178.7 (3)	N2—C9—C14—C13	−179.8 (4)
O3—N3—C5—C6	−179.5 (5)	C1—S1—C15—C16	−114.3 (3)
O4—N3—C5—C6	1.7 (7)	S1—C15—C16—C17	−65.9 (4)
O3—N3—C5—C4	2.3 (6)	C15—C16—C17—O1	−3.1 (14)
O4—N3—C5—C4	−176.5 (4)	C15—C16—C17—O5	173.2 (6)
C4—C5—C6—C7	−1.3 (7)	O1—C17—O5—C18	−3.9 (15)
N3—C5—C6—C7	−179.4 (4)	C16—C17—O5—C18	179.8 (6)
C5—C6—C7—C8	1.2 (7)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6*A*···O2^{i}	0.93	2.56	3.142 (5)	121
C10—H10*A*···O2^{ii}	0.93	2.39	3.167 (5)	140

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