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Ethyl 6′-cyano-7′-phenyl-1′,6′,7′,7a′-tetrahydro-3′*H*-spiro[indeno[1,2-*b*]quinoxaline-11,5′-pyrrolo-[1,2-c]thiazole-6′-carboxylate

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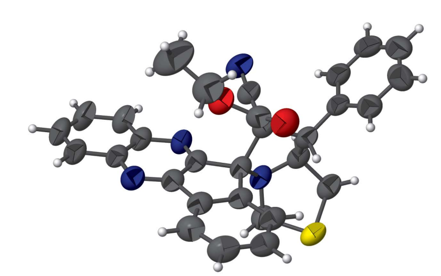
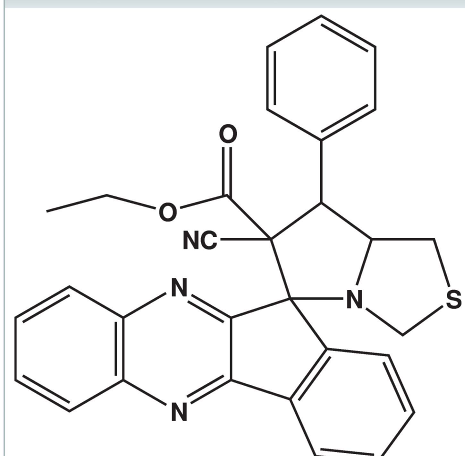
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{22}H_{22}ClN_4O_2S$, the angle between the mean planes of the indene ring and the quinoxaline ring system is 3.93 (11)°. The five-membered indene and thiazole rings both adopt envelope conformations while the pyrrole ring adopts a twisted conformation. The two acceptor O atoms form a chelated three-centred hydrogen bond with a phenyl C atom.

3D view



Chemical scheme



Structure description

Quinoxaline derivatives have attracted considerable attention due to their biological activities and use as anti-viral, anti-bacterial, anti-inflammatory, anti-protozoaol, anti cancer, anti depressant and anti-HIV agents. Drugs containing a quinoxaline core are under clinical trial for anticancer therapeutic purposes (Zhang *et al.*, 2013). Indeno-quinoxaline derivatives have found applications in dyes (Sehlstedt *et al.*, 1998) and as organic semiconductors (Gazit *et al.*, 1996). Moreover, thiazole derivatives are found to be antituberculous, bacteriostatic and fungistatic agents (Shao *et al.*, 2004). A search in the CSD (version 5.39, update, May 2018; Groom *et al.*, 2016) for structures of the title compound containing indene, quinoxaline pyrrolo and thiazole with no filters gave seven hits: DEHFUU (Muthuselvi *et al.*, 2017), DOPYO,(Sivakumar *et al.*, 2014), DUXPET (Malathi *et al.*,2015), FUQCAX (Hamzehloueian *et al.*, 2015), NIKSOR (Suhitha *et al.*, 2013*a*), NIKSUK (Suhitha *et al.*, 2013*b*) and RENZUI (Muthuselvi *et al.*, 2018). In view of the important biological activities of indenoquinoxaline-pyrolothiazole derivatives, the crystal structure of the title compound has been determined (Fig. 1).

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

D—H$\cdots$$A$	D—H	H$\cdots$$A$	$D$$\cdots$$A$	D—H$\cdots$$A$
C17—H17$B$$\cdots$N4^{i}	0.97	2.65	3.560 (4)	156
C21—H21$B$$\cdots$O1^{ii}	0.97	2.89	3.399 (3)	114
C27—H27$\cdots$O1^{iii}	0.93	2.90	3.562 (4)	129
C27—H27$\cdots$O2^{iii}	0.93	2.87	3.798 (4)	174
C18—H18$B$$\cdots$N2^{iv}	0.97	2.66	3.609 (4)	166

Symmetry codes: (i) $-x+1, y, -z+\frac{3}{2}$; (ii) $-x+1, y, -z+\frac{1}{2}$; (iii) $-x+1, -y+1, -z+1$; (iv) $-x+1, -y, -z+1$.

The five-membered thiazole ring (S1/C17/C16/N3/C18) adopts an envelope conformation on S1 with puckering parameters $Q(2)$ = 0.473 (2) Å and $\varphi(2)$ = 358.2 (2)°. The pyrrole ring (N3/C1/C19/C23/C16) adopts a twisted conformation on C19—C23 with puckering amplitude $Q(2)$ = 0.443 (3) Å and $\varphi(2)$ = 82.6 (3)°. The five-membered indene ring (C1–C5) adopts an envelope conformation on C1 with puckering parameters $Q(2)$ = 0.076 (3) Å and $\varphi(2)$ = 182 (2)°, but the six-membered rings of both indene and quinoxaline does not show any significant deviation from planarity. The mean planes of indene and quinoxaline make an angle 3.93 (11)°.

The mean plane through the quinoxaline ring system and the fused indene ring makes dihedral angles of 76.36 (6) and 54.94 (8)°, respectively, with the mean planes through the pyrrole and thiazole rings.

In the crystal, pairs of C17—H117$B$$\cdots$N4^{i} hydrogen bonds (Table 1) connect molecules into inversion dimers with an $R_2^2(14)$ motif while C21—H21$B$$\cdots$O1^{ii} hydrogen bonds form an $R_2^2(10)$ graph-set motif. Together, these interactions lead to the formation of chains running along the c-axis direction (Fig. 2). The O atoms O1 and O2 form a chelated three-centered hydrogen bond with the phenyl carbon atom C27, leading to a dimeric $R_2^2(18)$ motif. The C18—H18$B$$\cdots$N2^{iv} hydrogen bond forms an $R_2^2(24)$ graph-set motif. This C—H$\cdots$N hydrogen bond and the chelated three-centered C—H$\cdots$O hydrogen bonds lead to the formation of a linear chain extending along the b-axis direction (Fig. 3).

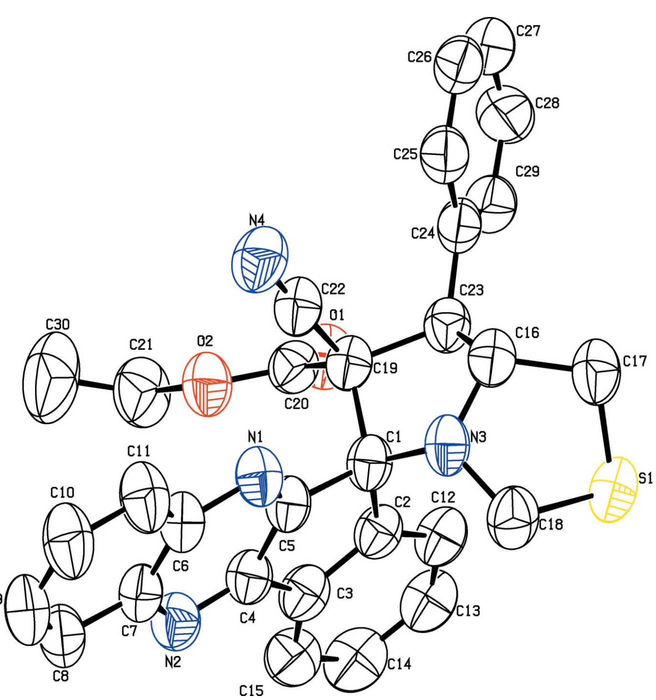


Figure 1
Displacement ellipsoid plot (50% probability level) of the title compound, showing the atom-labelling scheme. H atoms have been omitted for clarity.

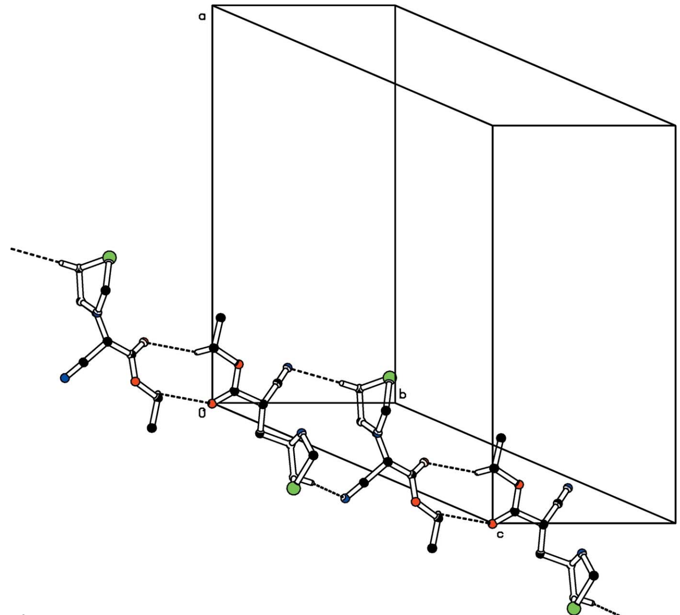


Figure 2
Part of the crystal structure of the title compound, showing the formation of $R_2^2(10)$ and $R_2^2(14)$ graph-set motifs. Dashed lines indicate hydrogen bonds. The fused indeno-quinoxaline rings and H atoms not involved in the hydrogen bonding have been omitted for the sake of clarity.

Synthesis and crystallization

Equimolar amounts of 11H-indeno[1,2-b]quinoxalin-11-one and thiazolidine-4-carboxylic acid were added to methanol

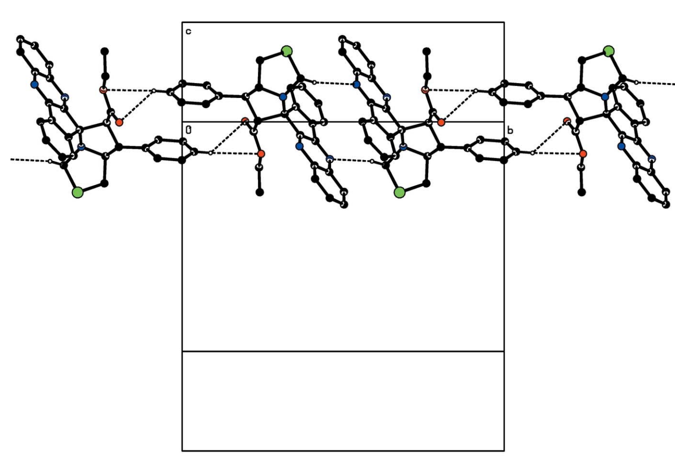


Figure 3
Part of the crystal structure of the title compound, showing the formation of $R_2^2(18)$ and $R_2^2(24)$ graph-set motifs. Dashed lines indicate hydrogen bonds. The H atoms not involved in the hydrogen bonding have been omitted for the sake of clarity.

(20 ml) and the mixture was refluxed in a water bath for 2 min. Then an equimolar amount of propyl (*E*)-2-cyano-3-(phenyl) acrylate was added to the reaction mixture and refluxing was continued until the completion of the reaction (monitored using TLC) after 4 h. The precipitated solid was filtered and washed with methanol to obtain the title compound. Colourless needle-shaped crystals were obtained by the slow evaporation of a chloroform solution.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{30}H_{24}N_4O_2S$
M_r	504.59
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	273
a, *b*, *c* (Å)	18.6131 (13), 18.2243 (13), 15.8867 (11)
β (°)	110.757 (1)
V (Å^3)	5039.2 (6)
Z	8
Radiation type	Mo *K*α
μ (mm^{-1})	0.16
Crystal size (mm)	0.30 × 0.16 × 0.12
Data collection	
Diffractometer	Bruker SMART APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)
T_{min}, T_{max}	0.95, 1.0
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	26271, 5092, 3836
R_{int}	0.028
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.622
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.064, 0.186, 1.03
No. of reflections	5092
No. of parameters	335
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.52, −0.16

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXS2013* (Sheldrick, 2008), *SHELXL2018* (Sheldrick, 2015), *PLUTON* (Spek, 2009) and *publCIF* (Westrip, 2010).

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full crystallographic data

IUCrData (2018). **3**, x181286 [https://doi.org/10.1107/S2414314618012865]

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Crystal data

$C_{30}H_{24}N_4O_2S$
M_r = 504.59
Monoclinic, $C2/c$
a = 18.6131 (13) Å
b = 18.2243 (13) Å
c = 15.8867 (11) Å
β = 110.757 (1)°
V = 5039.2 (6) Å^3
Z = 8
$F(000)$ = 2112
D_x = 1.330 Mg m^{-3}
D_m = 1.32 Mg m^{-3}
D_m measured by floatation method
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6051 reflections
θ = 1.5–26.5°
μ = 0.16 mm^{-1}
T = 273 K
Needle, colorless
0.30 × 0.16 × 0.12 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.95, T_{max} = 1.0
26271 measured reflections
5092 independent reflections
3836 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 26.3°, θ_{min} = 2.2°
h = −23→23
k = −22→22
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.186
S = 1.03
5092 reflections
335 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1079P)^2 + 2.3737P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}
S1	0.30934 (4)	0.17536 (4)	0.57840 (5)	0.0739 (3)
O1	0.45967 (11)	0.30451 (11)	0.37194 (12)	0.0762 (5)
O2	0.57726 (10)	0.25504 (11)	0.43424 (11)	0.0723 (5)
N1	0.61674 (11)	0.13563 (12)	0.64087 (13)	0.0621 (5)
N2	0.61166 (12)	0.04137 (12)	0.49401 (14)	0.0666 (5)
N3	0.45872 (10)	0.18686 (11)	0.61438 (12)	0.0598 (5)
N4	0.63289 (13)	0.31402 (15)	0.64698 (17)	0.0825 (7)
C1	0.48811 (12)	0.18165 (13)	0.54051 (14)	0.0548 (5)
C2	0.43822 (13)	0.14707 (13)	0.44885 (14)	0.0563 (5)
C3	0.48151 (13)	0.09497 (14)	0.42181 (15)	0.0612 (6)
C4	0.55572 (13)	0.08615 (13)	0.49236 (15)	0.0578 (5)
C5	0.56009 (12)	0.13355 (13)	0.56520 (15)	0.0562 (5)
C6	0.67664 (13)	0.08905 (14)	0.64557 (16)	0.0629 (6)
C7	0.67404 (13)	0.04323 (14)	0.57230 (17)	0.0622 (6)
C8	0.73716 (15)	−0.00236 (16)	0.5810 (2)	0.0765 (7)
H8	0.736470	−0.032498	0.533507	0.092*
C9	0.79906 (15)	−0.00253 (19)	0.6585 (2)	0.0869 (9)
H9	0.840694	−0.032686	0.663610	0.104*
C10	0.80104 (15)	0.0418 (2)	0.7304 (2)	0.0900 (9)
H10	0.843691	0.040567	0.783354	0.108*
C11	0.74084 (14)	0.08723 (18)	0.72407 (18)	0.0806 (8)
H11	0.742915	0.116967	0.772452	0.097*
C12	0.36429 (14)	0.16269 (15)	0.39147 (16)	0.0650 (6)
H12	0.334415	0.196494	0.408266	0.078*
C13	0.33503 (15)	0.12760 (16)	0.30874 (17)	0.0719 (7)
H13	0.285422	0.138216	0.270113	0.086*
C14	0.37851 (17)	0.07725 (18)	0.28311 (18)	0.0810 (8)
H14	0.358092	0.054641	0.227159	0.097*
C15	0.45188 (16)	0.05996 (16)	0.33932 (16)	0.0716 (7)
H15	0.480913	0.025485	0.322203	0.086*
C16	0.43303 (13)	0.26156 (14)	0.62393 (15)	0.0613 (6)
H16	0.469645	0.283697	0.678522	0.074*
C17	0.35336 (15)	0.25831 (17)	0.63304 (19)	0.0755 (7)
H17A	0.322730	0.300548	0.604378	0.091*
H17B	0.358505	0.257668	0.695971	0.091*
C18	0.40462 (15)	0.13219 (16)	0.62071 (19)	0.0725 (7)
H18A	0.417100	0.116742	0.682696	0.087*
H18B	0.405837	0.089559	0.584682	0.087*
C19	0.50524 (12)	0.26528 (13)	0.52728 (14)	0.0559 (5)

C20	0.50988 (14)	0.27817 (13)	0.43387 (16)	0.0595 (6)
C21	0.59318 (19)	0.2614 (2)	0.3500 (2)	0.0898 (9)
H21A	0.569101	0.221297	0.309738	0.108*
H21B	0.572803	0.307257	0.319989	0.108*
C22	0.57810 (14)	0.29091 (15)	0.59573 (16)	0.0628 (6)
C23	0.43634 (13)	0.30320 (13)	0.54228 (15)	0.0579 (6)
H23	0.390463	0.288851	0.491480	0.070*
C24	0.43508 (13)	0.38595 (14)	0.54682 (17)	0.0635 (6)
C25	0.48189 (15)	0.42620 (17)	0.6192 (2)	0.0792 (8)
H25	0.517107	0.402287	0.668255	0.095*
C26	0.47659 (19)	0.5021 (2)	0.6190 (3)	0.0985 (11)
H26	0.508978	0.529091	0.667254	0.118*
C27	0.4239 (2)	0.5372 (2)	0.5480 (3)	0.1001 (11)
H27	0.420269	0.588046	0.548416	0.120*
C28	0.3769 (2)	0.49888 (17)	0.4773 (3)	0.0904 (9)
H28	0.340960	0.523328	0.429366	0.108*
C29	0.38218 (16)	0.42342 (15)	0.4762 (2)	0.0731 (7)
H29	0.349685	0.397341	0.427102	0.088*
C30	0.6754 (2)	0.2591 (3)	0.3728 (3)	0.1403 (17)
H30A	0.698959	0.296744	0.415987	0.210*
H30B	0.687503	0.266864	0.319552	0.210*
H30C	0.694450	0.211981	0.398039	0.210*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0546 (4)	0.1003 (6)	0.0709 (4)	−0.0089 (3)	0.0272 (3)	0.0014 (3)
O1	0.0766 (12)	0.0963 (13)	0.0531 (9)	0.0020 (10)	0.0197 (9)	0.0065 (9)
O2	0.0684 (10)	0.0938 (13)	0.0640 (10)	0.0025 (9)	0.0349 (8)	0.0006 (9)
N1	0.0505 (10)	0.0813 (14)	0.0550 (11)	0.0075 (9)	0.0193 (9)	0.0018 (9)
N2	0.0626 (12)	0.0781 (14)	0.0654 (12)	−0.0012 (10)	0.0304 (10)	−0.0021 (10)
N3	0.0508 (10)	0.0833 (14)	0.0498 (10)	0.0048 (9)	0.0232 (8)	0.0061 (9)
N4	0.0566 (13)	0.1076 (19)	0.0755 (14)	−0.0109 (12)	0.0137 (11)	−0.0064 (13)
C1	0.0470 (11)	0.0719 (15)	0.0463 (11)	0.0013 (10)	0.0175 (9)	0.0042 (10)
C2	0.0551 (12)	0.0683 (14)	0.0481 (11)	−0.0080 (10)	0.0214 (10)	0.0027 (10)
C3	0.0610 (13)	0.0737 (15)	0.0513 (12)	−0.0078 (11)	0.0229 (10)	0.0045 (11)
C4	0.0575 (13)	0.0670 (14)	0.0559 (12)	−0.0020 (10)	0.0287 (10)	0.0029 (10)
C5	0.0505 (12)	0.0711 (15)	0.0512 (12)	0.0004 (10)	0.0231 (10)	0.0051 (10)
C6	0.0500 (12)	0.0808 (16)	0.0623 (13)	0.0050 (11)	0.0253 (11)	0.0062 (12)
C7	0.0518 (12)	0.0745 (15)	0.0683 (14)	0.0002 (11)	0.0310 (11)	0.0042 (12)
C8	0.0600 (15)	0.0912 (19)	0.0889 (18)	0.0045 (13)	0.0395 (14)	−0.0050 (15)
C9	0.0539 (15)	0.110 (2)	0.105 (2)	0.0155 (15)	0.0383 (15)	0.0020 (18)
C10	0.0512 (14)	0.133 (3)	0.0815 (18)	0.0188 (15)	0.0178 (13)	0.0002 (18)
C11	0.0555 (14)	0.118 (2)	0.0666 (15)	0.0141 (14)	0.0202 (12)	−0.0042 (15)
C12	0.0557 (13)	0.0815 (17)	0.0549 (13)	−0.0072 (12)	0.0159 (11)	0.0068 (11)
C13	0.0637 (15)	0.0923 (19)	0.0543 (13)	−0.0121 (13)	0.0142 (12)	0.0051 (13)
C14	0.0829 (19)	0.104 (2)	0.0505 (13)	−0.0182 (16)	0.0165 (13)	−0.0042 (14)
C15	0.0804 (17)	0.0837 (18)	0.0555 (14)	−0.0095 (14)	0.0299 (13)	−0.0073 (12)

C16	0.0507 (12)	0.0833 (16)	0.0500 (12)	−0.0045 (11)	0.0179 (10)	−0.0080 (11)
C17	0.0632 (15)	0.104 (2)	0.0678 (15)	−0.0002 (14)	0.0332 (12)	−0.0061 (14)
C18	0.0722 (16)	0.0829 (18)	0.0721 (15)	0.0038 (13)	0.0374 (13)	0.0158 (13)
C19	0.0482 (11)	0.0705 (15)	0.0502 (12)	−0.0030 (10)	0.0187 (9)	−0.0004 (10)
C20	0.0605 (13)	0.0682 (15)	0.0527 (12)	−0.0086 (11)	0.0237 (11)	−0.0053 (11)
C21	0.097 (2)	0.120 (3)	0.0687 (17)	−0.0065 (18)	0.0489 (16)	−0.0110 (16)
C22	0.0526 (13)	0.0817 (17)	0.0562 (13)	−0.0019 (12)	0.0219 (11)	−0.0003 (12)
C23	0.0475 (11)	0.0750 (15)	0.0510 (12)	−0.0037 (10)	0.0171 (9)	−0.0081 (10)
C24	0.0508 (12)	0.0759 (16)	0.0714 (15)	−0.0082 (11)	0.0310 (11)	−0.0120 (12)
C25	0.0595 (14)	0.090 (2)	0.095 (2)	−0.0110 (13)	0.0364 (14)	−0.0284 (16)
C26	0.0746 (19)	0.104 (3)	0.136 (3)	−0.0325 (18)	0.061 (2)	−0.056 (2)
C27	0.099 (2)	0.079 (2)	0.153 (3)	−0.0158 (19)	0.084 (3)	−0.020 (2)
C28	0.106 (2)	0.0700 (19)	0.117 (2)	0.0009 (17)	0.066 (2)	−0.0001 (18)
C29	0.0704 (16)	0.0769 (18)	0.0795 (17)	−0.0056 (13)	0.0358 (14)	−0.0029 (14)
C30	0.109 (3)	0.219 (5)	0.122 (3)	−0.036 (3)	0.078 (3)	−0.039 (3)

Geometric parameters (Å, º)

S1—C17	1.791 (3)	C13—H13	0.9300
S1—C18	1.836 (3)	C14—C15	1.377 (4)
O1—C20	1.192 (3)	C14—H14	0.9300
O2—C20	1.321 (3)	C15—H15	0.9300
O2—C21	1.475 (3)	C16—C23	1.523 (3)
N1—C5	1.288 (3)	C16—C17	1.541 (3)
N1—C6	1.382 (3)	C16—H16	0.9800
N2—C4	1.316 (3)	C17—H17A	0.9700
N2—C7	1.369 (3)	C17—H17B	0.9700
N3—C18	1.445 (3)	C18—H18A	0.9700
N3—C1	1.463 (3)	C18—H18B	0.9700
N3—C16	1.468 (3)	C19—C22	1.481 (3)
N4—C22	1.137 (3)	C19—C20	1.535 (3)
C1—C5	1.531 (3)	C19—C23	1.548 (3)
C1—C2	1.556 (3)	C21—C30	1.443 (5)
C1—C19	1.586 (3)	C21—H21A	0.9700
C2—C12	1.384 (3)	C21—H21B	0.9700
C2—C3	1.407 (3)	C23—C24	1.510 (4)
C3—C15	1.384 (3)	C23—H23	0.9800
C3—C4	1.447 (3)	C24—C25	1.382 (4)
C4—C5	1.423 (3)	C24—C29	1.383 (4)
C6—C11	1.389 (3)	C25—C26	1.387 (5)
C6—C7	1.419 (4)	C25—H25	0.9300
C7—C8	1.405 (3)	C26—C27	1.363 (5)
C8—C9	1.356 (4)	C26—H26	0.9300
C8—H8	0.9300	C27—C28	1.348 (5)
C9—C10	1.388 (4)	C27—H27	0.9300
C9—H9	0.9300	C28—C29	1.379 (4)
C10—C11	1.368 (4)	C28—H28	0.9300
C10—H10	0.9300	C29—H29	0.9300

C11—H11	0.9300	C30—H30A	0.9600
C12—C13	1.388 (4)	C30—H30B	0.9600
C12—H12	0.9300	C30—H30C	0.9600
C13—C14	1.377 (4)		

C17—S1—C18	88.14 (13)	C17—C16—H16	108.9
C20—O2—C21	117.8 (2)	C16—C17—S1	106.09 (18)
C5—N1—C6	114.2 (2)	C16—C17—H17A	110.5
C4—N2—C7	114.4 (2)	S1—C17—H17A	110.5
C18—N3—C1	118.6 (2)	C16—C17—H17B	110.5
C18—N3—C16	111.81 (18)	S1—C17—H17B	110.5
C1—N3—C16	111.78 (18)	H17A—C17—H17B	108.7
N3—C1—C5	111.94 (17)	N3—C18—S1	106.59 (18)
N3—C1—C2	120.54 (18)	N3—C18—H18A	110.4
C5—C1—C2	100.70 (18)	S1—C18—H18A	110.4
N3—C1—C19	101.18 (18)	N3—C18—H18B	110.4
C5—C1—C19	112.66 (17)	S1—C18—H18B	110.4
C2—C1—C19	110.27 (17)	H18A—C18—H18B	108.6
C12—C2—C3	118.7 (2)	C22—C19—C20	108.11 (18)
C12—C2—C1	131.1 (2)	C22—C19—C23	109.83 (18)
C3—C2—C1	110.03 (19)	C20—C19—C23	114.47 (19)
C15—C3—C2	121.4 (2)	C22—C19—C1	112.36 (19)
C15—C3—C4	129.3 (2)	C20—C19—C1	110.98 (18)
C2—C3—C4	109.3 (2)	C23—C19—C1	101.08 (17)
N2—C4—C5	122.9 (2)	O1—C20—O2	126.7 (2)
N2—C4—C3	128.0 (2)	O1—C20—C19	124.3 (2)
C5—C4—C3	109.0 (2)	O2—C20—C19	109.0 (2)
N1—C5—C4	124.7 (2)	C30—C21—O2	107.8 (3)
N1—C5—C1	125.1 (2)	C30—C21—H21A	110.1
C4—C5—C1	110.28 (19)	O2—C21—H21A	110.1
N1—C6—C11	119.0 (2)	C30—C21—H21B	110.1
N1—C6—C7	121.6 (2)	O2—C21—H21B	110.1
C11—C6—C7	119.4 (2)	H21A—C21—H21B	108.5
N2—C7—C8	119.0 (2)	N4—C22—C19	176.6 (3)
N2—C7—C6	122.1 (2)	C24—C23—C16	116.79 (19)
C8—C7—C6	118.9 (2)	C24—C23—C19	118.75 (19)
C9—C8—C7	120.2 (3)	C16—C23—C19	101.22 (18)
C9—C8—H8	119.9	C24—C23—H23	106.4
C7—C8—H8	119.9	C16—C23—H23	106.4
C8—C9—C10	120.8 (3)	C19—C23—H23	106.4
C8—C9—H9	119.6	C25—C24—C29	118.1 (3)
C10—C9—H9	119.6	C25—C24—C23	123.6 (3)
C11—C10—C9	120.6 (3)	C29—C24—C23	118.2 (2)
C11—C10—H10	119.7	C24—C25—C26	120.3 (3)
C9—C10—H10	119.7	C24—C25—H25	119.9
C10—C11—C6	120.2 (3)	C26—C25—H25	119.9
C10—C11—H11	119.9	C27—C26—C25	119.9 (3)
C6—C11—H11	119.9	C27—C26—H26	120.0

C2—C12—C13	119.6 (3)	C25—C26—H26	120.0
C2—C12—H12	120.2	C28—C27—C26	120.7 (3)
C13—C12—H12	120.2	C28—C27—H27	119.6
C14—C13—C12	120.8 (3)	C26—C27—H27	119.6
C14—C13—H13	119.6	C27—C28—C29	119.9 (4)
C12—C13—H13	119.6	C27—C28—H28	120.0
C15—C14—C13	120.8 (2)	C29—C28—H28	120.0
C15—C14—H14	119.6	C28—C29—C24	121.0 (3)
C13—C14—H14	119.6	C28—C29—H29	119.5
C14—C15—C3	118.6 (3)	C24—C29—H29	119.5
C14—C15—H15	120.7	C21—C30—H30A	109.5
C3—C15—H15	120.7	C21—C30—H30B	109.5
N3—C16—C23	105.12 (17)	H30A—C30—H30B	109.5
N3—C16—C17	109.5 (2)	C21—C30—H30C	109.5
C23—C16—C17	115.5 (2)	H30A—C30—H30C	109.5
N3—C16—H16	108.9	H30B—C30—H30C	109.5
C23—C16—H16	108.9		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C17—H17*B*···N4^{i}	0.97	2.65	3.560 (4)	156
C21—H21*B*···O1^{ii}	0.97	2.89	3.399 (3)	114
C27—H27···O1^{iii}	0.93	2.90	3.562 (4)	129
C27—H27···O2^{iii}	0.93	2.87	3.798 (4)	174
C18—H18*B*···N2^{iv}	0.97	2.66	3.609 (4)	166

Symmetry codes: (i) −*x*+1, *y*, −*z*+3/2; (ii) −*x*+1, *y*, −*z*+1/2; (iii) −*x*+1, −*y*+1, −*z*+1; (iv) −*x*+1, −*y*, −*z*+1.