research communications

Crystal structure of 3-benzyl-2-[(E)-2-(furan-2-yl)ethenyl]-2,3-dihydroquinazolin-4(1H)-one and 3-benzyl-2-[(E)-2-(thiophen-2-yl)ethenyl]-2,3-dihydroquinazolin-4(1H)-one from synchrotron X-ray diffraction

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The chiral title compounds, $C_{21}H_{18}N_2O_2$, (I), and $C_{21}H_{18}N_2OS$, (II) – products of the three-component reaction between benzylamine, isatoic anhydride and furyl- or thienyl-acrolein – are isostructural and form isomorphous racemic crystals. The tetrahydropyrimidine ring in (I) and (II) adopts a sofa conformation. The amino N atom has a trigonal–pyramidal geometry [sum of the bond angles is 347.0° for both (I) and (II)], whereas the amido N atom is flat [sum of the bond angles is 359.3° for both (I) and (II)]. The furyl- and thienylethenyl substituents in (I) and (II) are planar and the conformation about the bridging C=C bond is E. These bulky fragments occupy the axial position at the quaternary C atom of the tetrahydropyrimidine ring, apparently, due to steric reasons. In the crystals, molecules of (I) and (II) form hydrogen-bonded helicoidal chains propagating along [010] by strong intermolecular N—H⋯O hydrogen bonds.

1. Chemical context

The synthesis and chemistry of quinazoline and quinazolinone derivatives have remained at the focus of biochemical research over the past decade owing to their high and diverse physiological activities (for recent reviews, see: Jafari *et al.*, 2016; Wang & Gao, 2013; Selvam & Kumar, 2011). A large part of these studies has been aimed at the development of methods for the synthesis of 2-aryl-substituted quinazolines. However, 2-ethenylquinazolines are much more attractive synthons for subsequent modifications of the heterocyclic skeleton.

Two synthetic approaches A and B (Fig. 1) are known for 2-ethenylphenyl-substituted heterocycles (Mohammadpoor-Baltork *et al.*, 2011; Ramesh *et al.*, 2012; Cheng *et al.*, 2012; Ghorbani-Choghamarani & Norouzi, 2014; Zhang *et al.*, 2014, 2016; Deng *et al.*, 2015; Noori *et al.*, 2017; Alinezhad *et al.*, 2017). However, up to date, there is practically no information about the synthesis of 2-ethenylhetaryl-substituted quinazolines (Frackenpohl *et al.*, 2016; Zaytsev *et al.*, 2015; Celltech & Limited, 2004; Kundu & Chaudhuri, 2001). Taking into account the high biological activity of furan, thiophene, and pyrrole derivatives, it appeared very attractive to obtain
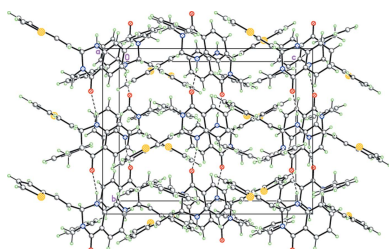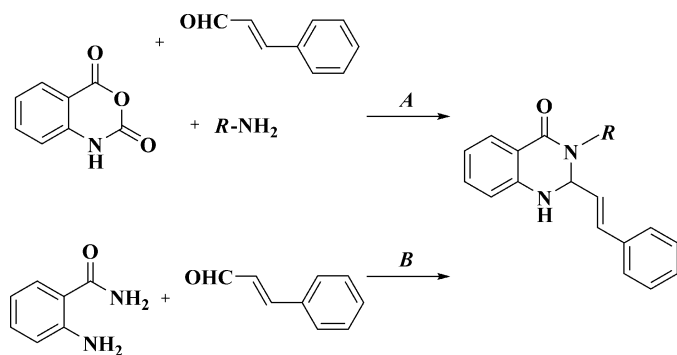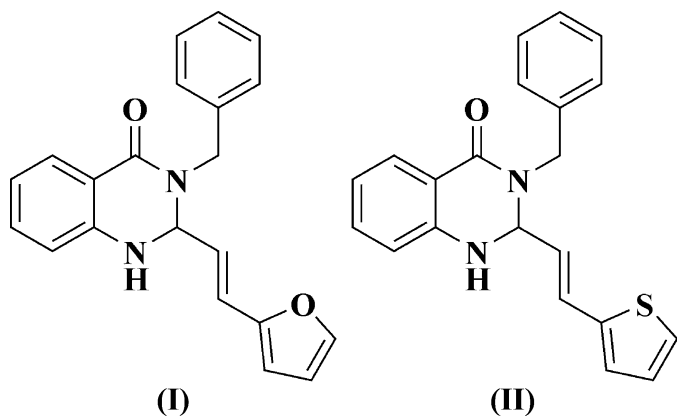
Figure 1
The two general methods, *A* and *B*, for the synthesis of 3-benzyl-2-[(*E*)-2-(2-aryl)ethenyl]-2,3-dihydroquinazolin-4(1*H*)-ones (I) and (II).

quinazolines of this type. It is well known that, for biological researches, the conformation of a molecule plays a key role. In this connection, the present work is aimed at revealing the conformational features of 2-ethenylhetaryl-substituted quinazolines.

Using method *A*, the three-component reaction between benzylamine, isatoic anhydride and furyl- or thienylacrolein in the presence of a catalytic quantity of *p*-TsOH afforded the 3-benzyl-2-[(*E*)-2-(furan-2-yl)ethenyl]-2,3-dihydroquinazolin-4(1*H*)-one (I) and 3-benzyl-2-[(*E*)-2-(thiophen-2-yl)ethenyl]-2,3-dihydroquinazolin-4(1*H*)-one (II) in moderate yields.

Figure 2
The molecular structure of (I). Displacement ellipsoids are shown at the 50% probability level. H atoms are presented as small spheres of arbitrary radius.

(II)]. The furyl- and thienyl-ethenyl substituents in (I) and (II) are planar and have the *E*-conformation at the C9=C10 double bond. Remarkably, these bulky fragments occupy the

(I)   **(II)**

2. Structural commentary

Compounds (I), $C_{21}H_{18}N_2O_2$, and (II), $C_{21}H_{18}N_2OS$ – the products of the three-component reaction between benzylamine, isatoic anhydride and furyl- or thienyl-acrolein are isostructural and crystallize in the orthorhombic space group *Pbca* (Figs. 2 and 3).

The tetrahydropyrimidine ring in (I) and (II) adopts a *sofa* conformation, with the C2 carbon atom deviating from the mean plane of the other atoms of the ring by 0.526 (1) and 0.528 (2) Å for (I) and (II), respectively. The nitrogen N1 atom has a trigonal-pyramidal geometry [sum of the bond angles is 347° for both (I) and (II)], whereas the nitrogen N3 atom is flattened [sum of the bond angles is 359.3° for both (I) and
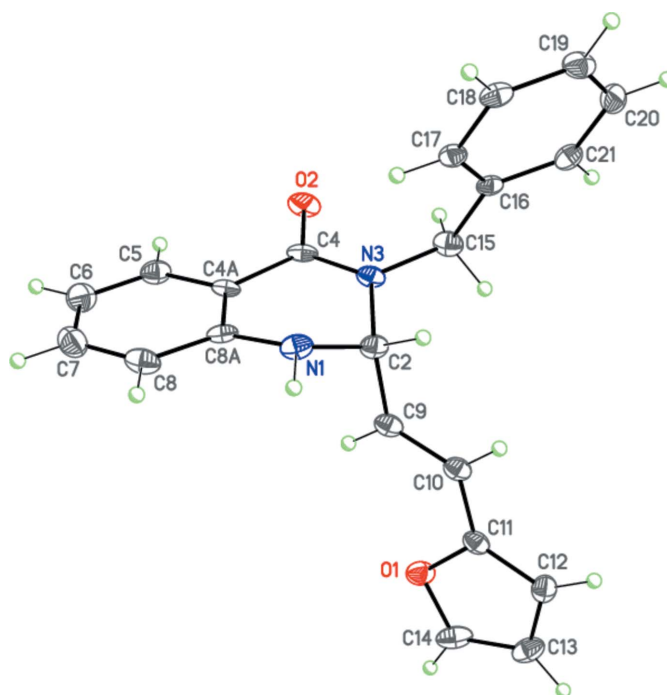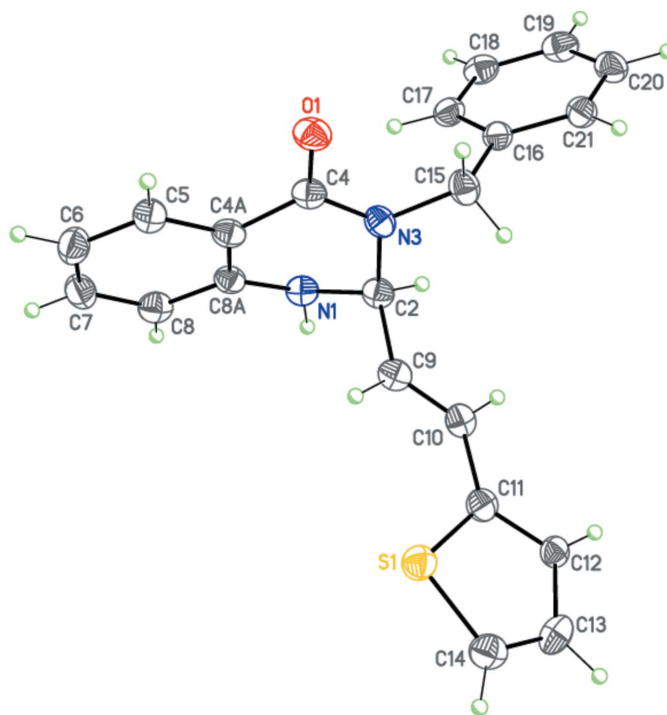

Figure 3
The molecular structure of (II). Displacement ellipsoids are shown at the 50% probability level. H atoms are presented as small spheres of arbitrary radius.
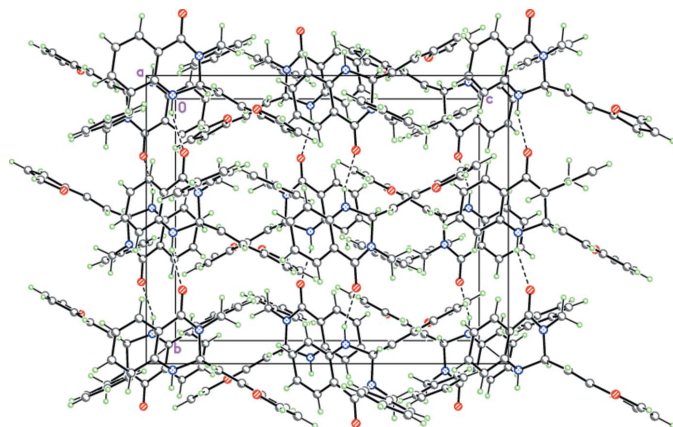
Figure 4
The crystal structure of (I), demonstrating the hydrogen-bonded helicoidal chains propagating in the [010] direction. Dashed lines indicate the intermolecular N—H···O hydrogen bonds.

axial position at the quaternary C2 carbon atom of the tetrahydropyrimidine ring, apparently, due to the steric interaction with the benzyl substituent.

The molecules of (I) and (II) possess an asymmetric center at the C2 carbon atom. The crystals of (I) and (II) are racemates.

3. Supramolecular features

In the crystals of (I) and (II), molecules form hydrogen-bonded helicoidal chains propagating along the [010] direction by strong intermolecular N—H···O hydrogen bonds (Tables 1 and 2, Figs. 4 and 5).

4. Synthesis and crystallization

3-Benzyl-2-[(E)-2-(2-aryl)ethenyl]-2,3-dihydroquinazolin-4-ones (I) and (II) were synthesized using a method similar to the recently described procedure (Fig. 6) (Zaytsev et al., 2017).
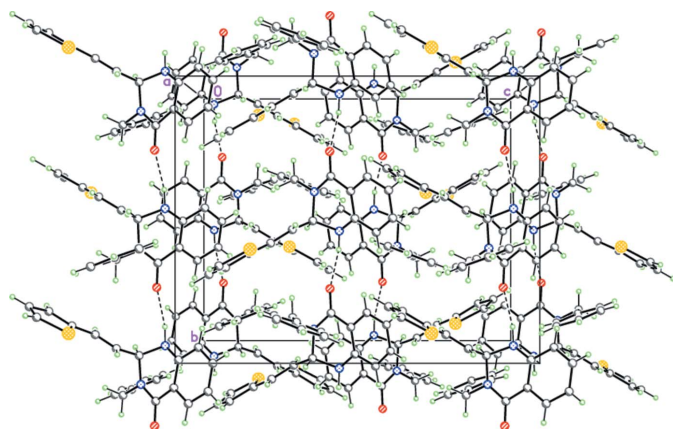

Figure 5
The crystal structure of (II), demonstrating the hydrogen-bonded helicoidal chains propagating in the [010] direction. Dashed lines indicate the intermolecular N—H···O hydrogen bonds.

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2[i]	0.897 (15)	2.111 (15)	2.9557 (14)	156.7 (12)

Symmetry code: (i) $-x + \frac{3}{2}, y - \frac{1}{2}, z$.

Table 2
Hydrogen-bond geometry (Å, °) for (II).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1[i]	0.87 (3)	2.14 (3)	2.978 (2)	161 (2)

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

General procedure. p-TsOH (0.79 g, 4.6 mmol) was added to a mixture of isatoic anhydride (1.5 g, 9.2 mmol), benzylamine (1.2 mL, 11.0 mmol), and furyl- or thienylacrolein (9.2 mmol) in 50 mL EtOH. The reaction mixture was heated under reflux for 4 h. The progress of the reaction was monitored by TLC. When the reaction completed, the mixture was diluted with H_2O (100 mL) and extracted with EtOAc (3 × 50 mL). The organic layers were combined, dried (MgSO$_4$), concentrated in vacuo and the residue was purified by column chromatography on SiO$_2$ (3 × 20 cm) using hexane and then EtOAc/hexane (1/10→1/5) mixtures as eluent. The resulting product was recrystallized from a mixture of hexane–EtOAc [for (I)] or EtOAc–EtOH [for (II)] to afford the analytically pure samples of the target products.

3-Benzyl-2-[(E)-2-(furan-2-yl)ethenyl]-2,3-dihydroquinazolin-4(1H)-one (I). Colourless prisms. Yield is 2.31 g (76%). M.p. = 427.1 K (hexane–EtOAc). IR (KBr), ν (cm^{-1}): 3376, 1645, 1611. ^{1}H NMR (CDCl$_3$, 600.2 MHz, 301 K): δ = 3.86 (d, 1H, CH$_2$N, J = 15.1), 4.61 (br s, 1H, NH), 4.98 (br d, 1H, H2, J = 5.5), 5.59 (d, 1H, CH$_2$N, J = 15.1), 6.24 (d, 1H, H3, furyl, J = 3.1), 6.25 (d, 1H, CH=CH, J = 6.2), 6.34 (dd, 1H, H4, furyl, J = 2.1, J = 3.1), 6.59 (d, 1H, H8, J = 8.2), 6.83 (t, 1H, H6, J = 7.6), 7.24–7.34 (m, 7H, HAr), 7.96 (dd, 1H, H5, J = 1.4, J = 7.6). ^{13}C NMR (CDCl$_3$, 100 MHz, 301 K): δ = 46.7 (CH$_2$N), 69.8 (C2), 109.9, 111.5, 114.8, 119.1, 121.1, 123.6, 127.5, 127.9, 128.7, 128.7, 133.6, 115.7, 136.9, 145.4, 151.1, 142.7 (CAr, CH=CH), 162.9 (NCO). MS (EI, 70 eV): m/z = 330 $[M]^+$ (93), 239 (100), 197 (71), 170 (20), 160 (19), 120 (40), 106 (55), 91 (81), 76 (58), 65 (45), 51 (37), 43 (20).

3-Benzyl-2-[(E)-2-(thiophen-2-yl)ethenyl]-2,3-dihydroquinazolin-4(1H)-one (II). Yellow prisms. Yield is 2.39 g (75%). M.p. = 434.1–435.1 K (EtOAc–EtOH). IR (KBr), ν
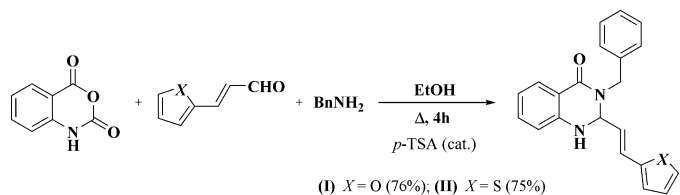

Figure 6
Syntheses of 3-benzyl-2-[(E)-2-(furan-2-yl)ethenyl]-2,3-dihydroquinazolin-4(1H)-one (I) and 3-benzyl-2-[(E)-2-(thiophen-2-yl)ethenyl]-2,3-dihydroquinazolin-4(1H)-one (II).

Table 3
Experimental details.

	(I)	(II)
Crystal data		
Chemical formula	$C_{21}H_{18}N_2O_2$	$C_{21}H_{18}N_2OS$
M_r	330.37	346.43
Crystal system, space group	Orthorhombic, $Pbca$	Orthorhombic, $Pbca$
Temperature (K)	100	100
a, b, c (Å)	14.292 (3), 13.729 (3), 17.230 (3)	14.245 (3), 13.855 (3), 17.629 (4)
V (Å^3)	3380.8 (12)	3479.3 (13)
Z	8	8
Radiation type	Synchrotron, $\lambda = 0.96260$ Å	Synchrotron, $\lambda = 0.96260$ Å
μ (mm^{-1})	0.17	0.44
Crystal size (mm)	$0.30 \times 0.25 \times 0.15$	$0.30 \times 0.25 \times 0.25$
Data collection		
Diffractometer	Rayonix SX165 CCD	Rayonix SX165 CCD
Absorption correction	Multi-scan (*SCALA*; Evans, 2006)	Multi-scan (*SCALA*; Evans, 2006)
T_{min}, T_{max}	0.940, 0.970	0.870, 0.890
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	34783, 3705, 3017	20322, 3594, 3024
R_{int}	0.079	0.064
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.646	0.647
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.042, 0.112, 1.08	0.050, 0.147, 1.08
No. of reflections	3705	3594
No. of parameters	230	217
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.28, −0.17	0.71, −0.72

Computer programs: *Marccd* (Doyle, 2011), *iMOSFLM* (Battye *et al.*, 2011), *SHELXT* (Sheldrick, 2015), *SHELXL2014* (Sheldrick, 2015) and *SHELXTL* (Sheldrick, 2015).

(cm^{-1}): 3306, 1625, 1506. ^{1}H NMR (DMSO, 600.2 MHz, 301 K): δ = 4.05 (*d*, 1H, CH$_2$N, *J* = 15.8), 5.15-5.17 (*m*, 2H, H2, CH$_2$N), 6.00 (*dd*, 1H, CH=CH, *J* = 6.8, *J* = 15.1), 6.69–6.76 (*m*, 3H, H6, H8, CH=CH), 6.96 (*dd*, 1H, H4, thienyl, *J* = 3.4, *J* = 5.2), 7.07 (*br d*, 1H, H3, thienyl, *J* = 3.4), 7.07 (*br s*, 1H, NH), 7.23–7.32 (*m*, 6H, HAr), 7.38 (*br d*, 1H, H2, thienyl, *J* = 5.2), 7.66 (*dd*, 1H, H5, *J* = 1.4, *J* = 8.2). ^{13}C NMR (DMSO, 150.9 MHz, 301 K): δ = 47.0 (CH$_2$N), 69.6 (C2), 115.1, 115.2, 118.0, 125.7 (2C), 126.4, 127.7, 127.9, 128.1, 128.3, 128.4, 129.0, 134.0, 138.3, 140.8, 147.1 (CAr, CH=CH), 162.4 (NCO). MS (EI, 70 eV): *m*/*z* = 346 [*M*]$^+$ (76), 255 (100), 237 (93), 213 (37), 106 (14), 91 (99), 65 (13).

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. X-ray diffraction studies were carried out on the "Belok" beamline of the National Research Center "Kurchatov Institute" (Moscow, Russian Federation) using a Rayonix SX165 CCD detector. A total of 360 images for each compounds were collected using an oscillation range of 1.0° (*φ* scan mode, two different crystal orientations) and corrected for absorption using the *SCALA* program (Evans, 2006). The data were indexed, integrated and scaled using the utility *iMOSFLM* in the *CCP4* program (Battye *et al.*, 2011).

The hydrogen atoms of the amino groups were localized in difference-Fourier maps and refined isotropically with fixed displacement parameters [$U_{iso}(H) = 1.2U_{eq}(N)$]. The other hydrogen atoms were placed in calculated positions with C—

H = 0.95–1.00 Å and refined in the riding model with fixed isotropic displacement parameters [$U_{iso}(H) = 1.2U_{eq}(C)$].

A relatively large number of reflections (a few dozen) were omitted due to the following reasons: (1) In order to achieve better I/σ statistics for high-angle reflections we selected a larger exposure time, which resulted in some intensity overloads in the low-angle part of the area. These corrupted intensities were excluded from final steps of the refinement. (2) In the current setup of the instrument, the low-temperature device eclipses a small region of the detector near its high-angle limit. This resulted in zero intensity of some reflections. (3) In the case of (II), the quality of the single crystal chosen for the diffraction experiment was far from perfect. Some systematic intensity deviations can be due to extinction and defects present in the crystal.

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supporting information

Crystal structure of 3-benzyl-2-[(*E*)-2-(furan-2-yl)ethenyl]-2,3-dihydro-quinazolin-4(1*H*)-one and 3-benzyl-2-[(*E*)-2-(thiophen-2-yl)ethenyl]-2,3-di-hydroquinazolin-4(1*H*)-one from synchrotron X-ray diffraction

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Computing details

For both structures, data collection: *Marccd* (Doyle, 2011); cell refinement: *iMOSFLM* (Battye *et al.*, 2011); data reduction: *iMOSFLM* (Battye *et al.*, 2011); program(s) used to solve structure: SHELXT (Sheldrick, 2015); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *SHELXTL* (Sheldrick, 2015); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2015).

3-Benzyl-2-[(*E*)-2-(furan-2-yl)ethenyl]-2,3-dihydroquinazolin-4(1*H*)-one (I)

Crystal data

$C_{21}H_{18}N_2O_2$	$D_x = 1.298$ Mg m^{-3}
$M_r = 330.37$	Synchrotron radiation, $\lambda = 0.96260$ Å
Orthorhombic, *Pbca*	Cell parameters from 600 reflections
$a = 14.292$ (3) Å	$\theta = 3.0$–$36.0°$
$b = 13.729$ (3) Å	$\mu = 0.17$ mm^{-1}
$c = 17.230$ (3) Å	$T = 100$ K
$V = 3380.8$ (12) Å^3	Prism, colourless
$Z = 8$	$0.30 \times 0.25 \times 0.15$ mm
$F(000) = 1392$	

Data collection

Rayonix SX165 CCD diffractometer	3705 independent reflections
/f scan	3017 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (Scala; Evans, 2006)	$R_{int} = 0.079$
	$\theta_{max} = 38.5°$, $\theta_{min} = 3.2°$
$T_{min} = 0.940$, $T_{max} = 0.970$	$h = -18 \rightarrow 18$
34783 measured reflections	$k = -17 \rightarrow 17$
	$l = -21 \rightarrow 21$

Refinement

Refinement on F^2	Primary atom site location: difference Fourier map
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.042$	
$wR(F^2) = 0.112$	Hydrogen site location: mixed
$S = 1.08$	H atoms treated by a mixture of independent and constrained refinement
3705 reflections	
230 parameters	
0 restraints	

$w = 1/[\sigma^2(F_o^2) + (0.0539P)^2 + 0.539P]$
  where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.28$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ e Å^{-3}

Extinction correction: SHELXL2014
(Sheldrick, 2015),
$Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0041 (8)

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 (Å^2)

	x	y	z	$U_{iso}*/U_{eq}$
O1	0.94874 (5)	0.38755 (6)	0.80431 (5)	0.0290 (2)
O2	0.78370 (6)	0.74574 (6)	0.58408 (5)	0.0324 (2)
N1	0.75445 (7)	0.45360 (8)	0.55253 (6)	0.0259 (3)
H1	0.7542 (10)	0.3883 (11)	0.5507 (8)	0.031*
C2	0.73864 (8)	0.49053 (9)	0.63117 (7)	0.0245 (3)
H2	0.6772	0.4641	0.6493	0.029*
N3	0.72977 (6)	0.59857 (7)	0.62784 (6)	0.0241 (2)
C4	0.78346 (8)	0.65486 (9)	0.57961 (7)	0.0243 (3)
C4A	0.83803 (7)	0.60140 (8)	0.51944 (7)	0.0239 (3)
C5	0.89993 (8)	0.65246 (9)	0.47069 (8)	0.0287 (3)
H5	0.9115	0.7196	0.4800	0.034*
C6	0.94453 (8)	0.60605 (10)	0.40899 (8)	0.0336 (3)
H6	0.9863	0.6409	0.3763	0.040*
C7	0.92651 (9)	0.50687 (10)	0.39610 (8)	0.0343 (3)
H7	0.9564	0.4747	0.3541	0.041*
C8	0.86562 (8)	0.45466 (9)	0.44362 (7)	0.0296 (3)
H8	0.8545	0.3875	0.4338	0.036*
C8A	0.82023 (7)	0.50135 (9)	0.50644 (7)	0.0240 (3)
C9	0.81224 (8)	0.45883 (8)	0.68936 (7)	0.0243 (3)
H9	0.8760	0.4743	0.6798	0.029*
C10	0.78969 (8)	0.40943 (9)	0.75408 (7)	0.0253 (3)
H10	0.7251	0.3963	0.7618	0.030*
C11	0.85346 (8)	0.37393 (9)	0.81353 (7)	0.0252 (3)
C12	0.83634 (9)	0.32594 (9)	0.88182 (7)	0.0295 (3)
H12	0.7769	0.3077	0.9017	0.035*
C13	0.92549 (9)	0.30860 (9)	0.91761 (8)	0.0328 (3)
H13	0.9367	0.2768	0.9657	0.039*
C14	0.99049 (9)	0.34671 (9)	0.86917 (8)	0.0321 (3)
H14	1.0560	0.3456	0.8784	0.039*
C15	0.67156 (8)	0.64346 (9)	0.68802 (7)	0.0271 (3)
H15A	0.6881	0.7133	0.6921	0.032*
H15B	0.6860	0.6125	0.7385	0.032*
C16	0.56621 (8)	0.63468 (8)	0.67274 (7)	0.0232 (3)
C17	0.52921 (8)	0.59729 (9)	0.60354 (7)	0.0255 (3)

H17	0.5702	0.5750	0.5639	0.031*
C18	0.43186 (8)	0.59258 (9)	0.59243 (8)	0.0287 (3)
H18	0.4074	0.5664	0.5456	0.034*
C19	0.37128 (8)	0.62615 (9)	0.64965 (8)	0.0319 (3)
H19	0.3055	0.6233	0.6418	0.038*
C20	0.40750 (9)	0.66416 (9)	0.71896 (8)	0.0316 (3)
H20	0.3663	0.6876	0.7580	0.038*
C21	0.50438 (8)	0.66754 (9)	0.73049 (7)	0.0272 (3)
H21	0.5286	0.6923	0.7779	0.033*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0247 (4)	0.0273 (5)	0.0350 (5)	−0.0009 (3)	−0.0026 (4)	0.0020 (4)
O2	0.0333 (5)	0.0183 (5)	0.0457 (6)	0.0014 (3)	0.0002 (4)	−0.0013 (4)
N1	0.0288 (5)	0.0170 (5)	0.0319 (6)	−0.0020 (4)	−0.0042 (4)	−0.0008 (4)
C2	0.0222 (5)	0.0201 (6)	0.0311 (7)	−0.0013 (4)	−0.0017 (5)	0.0008 (5)
N3	0.0208 (5)	0.0193 (5)	0.0322 (6)	0.0012 (4)	−0.0011 (4)	−0.0016 (4)
C4	0.0208 (5)	0.0188 (6)	0.0335 (7)	0.0010 (4)	−0.0060 (5)	0.0002 (5)
C4A	0.0200 (5)	0.0213 (6)	0.0303 (7)	0.0016 (4)	−0.0045 (5)	0.0009 (5)
C5	0.0231 (5)	0.0247 (7)	0.0385 (7)	0.0003 (5)	−0.0042 (5)	0.0036 (5)
C6	0.0256 (6)	0.0383 (8)	0.0370 (8)	0.0006 (5)	0.0015 (5)	0.0044 (6)
C7	0.0283 (6)	0.0421 (8)	0.0326 (7)	0.0059 (6)	−0.0002 (5)	−0.0057 (6)
C8	0.0274 (6)	0.0263 (7)	0.0351 (7)	0.0033 (5)	−0.0062 (5)	−0.0055 (5)
C8A	0.0215 (5)	0.0219 (6)	0.0285 (7)	0.0018 (4)	−0.0075 (5)	0.0007 (5)
C9	0.0214 (5)	0.0212 (6)	0.0305 (7)	−0.0006 (4)	−0.0013 (5)	−0.0027 (5)
C10	0.0224 (5)	0.0225 (6)	0.0311 (7)	0.0001 (4)	−0.0002 (5)	−0.0031 (5)
C11	0.0248 (5)	0.0220 (6)	0.0289 (7)	−0.0002 (5)	0.0008 (5)	−0.0042 (5)
C12	0.0326 (6)	0.0285 (7)	0.0274 (7)	−0.0013 (5)	0.0018 (5)	−0.0019 (5)
C13	0.0430 (7)	0.0279 (7)	0.0276 (7)	−0.0010 (6)	−0.0090 (6)	−0.0003 (5)
C14	0.0308 (6)	0.0262 (7)	0.0394 (8)	0.0004 (5)	−0.0122 (6)	0.0010 (6)
C15	0.0234 (6)	0.0266 (7)	0.0312 (7)	0.0010 (5)	−0.0025 (5)	−0.0047 (5)
C16	0.0232 (5)	0.0192 (6)	0.0273 (6)	0.0000 (4)	−0.0018 (5)	0.0032 (5)
C17	0.0263 (6)	0.0234 (6)	0.0268 (7)	0.0019 (5)	−0.0015 (5)	0.0021 (5)
C18	0.0287 (6)	0.0253 (7)	0.0320 (7)	−0.0016 (5)	−0.0070 (5)	0.0049 (5)
C19	0.0200 (5)	0.0332 (7)	0.0426 (8)	−0.0018 (5)	−0.0019 (5)	0.0100 (6)
C20	0.0275 (6)	0.0312 (7)	0.0360 (8)	0.0004 (5)	0.0090 (5)	0.0063 (6)
C21	0.0296 (6)	0.0246 (7)	0.0274 (7)	−0.0016 (5)	0.0018 (5)	0.0033 (5)

Geometric parameters (Å, º)

O1—C11	1.3836 (14)	C9—H9	0.9500
O1—C14	1.3854 (16)	C10—C11	1.4551 (17)
O2—C4	1.2501 (15)	C10—H10	0.9500
N1—C8A	1.3943 (16)	C11—C12	1.3707 (18)
N1—C2	1.4643 (17)	C12—C13	1.4354 (18)
N1—H1	0.897 (15)	C12—H12	0.9500
C2—N3	1.4898 (16)	C13—C14	1.3540 (19)

C2—C9	1.5169 (16)	C13—H13	0.9500
C2—H2	1.0000	C14—H14	0.9500
N3—C4	1.3699 (16)	C15—C16	1.5334 (16)
N3—C15	1.4653 (15)	C15—H15A	0.9900
C4—C4A	1.4905 (17)	C15—H15B	0.9900
C4A—C5	1.4069 (17)	C16—C17	1.4017 (17)
C4A—C8A	1.4149 (17)	C16—C21	1.4051 (17)
C5—C6	1.3938 (19)	C17—C18	1.4058 (16)
C5—H5	0.9500	C17—H17	0.9500
C6—C7	1.403 (2)	C18—C19	1.3907 (18)
C6—H6	0.9500	C18—H18	0.9500
C7—C8	1.3934 (19)	C19—C20	1.4023 (19)
C7—H7	0.9500	C19—H19	0.9500
C8—C8A	1.4154 (17)	C20—C21	1.3996 (17)
C8—H8	0.9500	C20—H20	0.9500
C9—C10	1.3445 (17)	C21—H21	0.9500
C11—O1—C14	106.06 (9)	C9—C10—H10	116.5
C8A—N1—C2	117.92 (10)	C11—C10—H10	116.5
C8A—N1—H1	116.9 (9)	C12—C11—O1	109.83 (10)
C2—N1—H1	112.2 (9)	C12—C11—C10	130.80 (11)
N1—C2—N3	108.80 (9)	O1—C11—C10	119.37 (10)
N1—C2—C9	113.91 (9)	C11—C12—C13	106.86 (11)
N3—C2—C9	111.72 (9)	C11—C12—H12	126.6
N1—C2—H2	107.4	C13—C12—H12	126.6
N3—C2—H2	107.4	C14—C13—C12	106.27 (11)
C9—C2—H2	107.4	C14—C13—H13	126.9
C4—N3—C15	120.66 (10)	C12—C13—H13	126.9
C4—N3—C2	122.51 (9)	C13—C14—O1	110.99 (11)
C15—N3—C2	116.09 (10)	C13—C14—H14	124.5
O2—C4—N3	121.82 (11)	O1—C14—H14	124.5
O2—C4—C4A	122.20 (11)	N3—C15—C16	113.75 (10)
N3—C4—C4A	115.92 (10)	N3—C15—H15A	108.8
C5—C4A—C8A	120.15 (11)	C16—C15—H15A	108.8
C5—C4A—C4	119.93 (11)	N3—C15—H15B	108.8
C8A—C4A—C4	119.61 (10)	C16—C15—H15B	108.8
C6—C5—C4A	121.02 (12)	H15A—C15—H15B	107.7
C6—C5—H5	119.5	C17—C16—C21	118.87 (11)
C4A—C5—H5	119.5	C17—C16—C15	123.05 (11)
C5—C6—C7	118.70 (12)	C21—C16—C15	118.07 (11)
C5—C6—H6	120.6	C16—C17—C18	120.40 (11)
C7—C6—H6	120.6	C16—C17—H17	119.8
C8—C7—C6	121.38 (12)	C18—C17—H17	119.8
C8—C7—H7	119.3	C19—C18—C17	120.28 (12)
C6—C7—H7	119.3	C19—C18—H18	119.9
C7—C8—C8A	120.18 (12)	C17—C18—H18	119.9
C7—C8—H8	119.9	C18—C19—C20	119.82 (11)
C8A—C8—H8	119.9	C18—C19—H19	120.1

N1—C8A—C4A	119.18 (11)	C20—C19—H19	120.1
N1—C8A—C8	122.12 (11)	C21—C20—C19	119.90 (12)
C4A—C8A—C8	118.57 (11)	C21—C20—H20	120.1
C10—C9—C2	121.78 (10)	C19—C20—H20	120.1
C10—C9—H9	119.1	C20—C21—C16	120.72 (12)
C2—C9—H9	119.1	C20—C21—H21	119.6
C9—C10—C11	127.06 (11)	C16—C21—H21	119.6
C8A—N1—C2—N3	45.76 (13)	C7—C8—C8A—C4A	0.11 (17)
C8A—N1—C2—C9	−79.59 (13)	N1—C2—C9—C10	−122.41 (12)
N1—C2—N3—C4	−38.41 (13)	N3—C2—C9—C10	113.81 (12)
C9—C2—N3—C4	88.20 (13)	C2—C9—C10—C11	179.09 (11)
N1—C2—N3—C15	151.40 (9)	C14—O1—C11—C12	−0.15 (13)
C9—C2—N3—C15	−81.99 (12)	C14—O1—C11—C10	179.98 (10)
C15—N3—C4—O2	−1.24 (16)	C9—C10—C11—C12	177.81 (13)
C2—N3—C4—O2	−171.00 (10)	C9—C10—C11—O1	−2.35 (18)
C15—N3—C4—C4A	−178.63 (9)	O1—C11—C12—C13	0.14 (14)
C2—N3—C4—C4A	11.61 (15)	C10—C11—C12—C13	179.99 (12)
O2—C4—C4A—C5	6.86 (17)	C11—C12—C13—C14	−0.07 (14)
N3—C4—C4A—C5	−175.76 (10)	C12—C13—C14—O1	−0.02 (15)
O2—C4—C4A—C8A	−166.71 (11)	C11—O1—C14—C13	0.10 (14)
N3—C4—C4A—C8A	10.66 (15)	C4—N3—C15—C16	111.21 (12)
C8A—C4A—C5—C6	0.12 (17)	C2—N3—C15—C16	−78.40 (13)
C4—C4A—C5—C6	−173.42 (11)	N3—C15—C16—C17	−6.96 (16)
C4A—C5—C6—C7	0.08 (18)	N3—C15—C16—C21	174.31 (10)
C5—C6—C7—C8	−0.18 (19)	C21—C16—C17—C18	−0.21 (17)
C6—C7—C8—C8A	0.08 (19)	C15—C16—C17—C18	−178.93 (11)
C2—N1—C8A—C4A	−27.67 (15)	C16—C17—C18—C19	0.82 (18)
C2—N1—C8A—C8	156.49 (11)	C17—C18—C19—C20	−0.48 (18)
C5—C4A—C8A—N1	−176.20 (10)	C18—C19—C20—C21	−0.45 (18)
C4—C4A—C8A—N1	−2.63 (15)	C19—C20—C21—C16	1.06 (18)
C5—C4A—C8A—C8	−0.21 (16)	C17—C16—C21—C20	−0.73 (17)
C4—C4A—C8A—C8	173.35 (10)	C15—C16—C21—C20	178.06 (11)
C7—C8—C8A—N1	175.97 (11)		

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2ⁱ	0.897 (15)	2.111 (15)	2.9557 (14)	156.7 (12)

Symmetry code: (i) −*x*+3/2, *y*−1/2, *z*.

3-Benzyl-2-[(*E*)-2-(thiophen-2-yl)ethenyl]-2,3-dihydroquinazolin-4(1*H*)-one (II)

Crystal data

$C_{21}H_{18}N_2OS$	*b* = 13.855 (3) Å
M_r = 346.43	*c* = 17.629 (4) Å
Orthorhombic, *Pbca*	*V* = 3479.3 (13) Å³
a = 14.245 (3) Å	*Z* = 8

$F(000) = 1456$

$D_x = 1.323$ Mg m^{-3}

Synchrotron radiation, $\lambda = 0.96260$ Å

Cell parameters from 600 reflections

$\theta = 3.0–33.0°$

$\mu = 0.44$ mm^{-1}

$T = 100$ K

Prism, yellow

$0.30 \times 0.25 \times 0.25$ mm

Data collection

Rayonix SX165 CCD
    diffractometer

φ scan

Absorption correction: multi-scan
    (*Scala*; Evans, 2006)

$T_{min} = 0.870$, $T_{max} = 0.890$

20322 measured reflections

3594 independent reflections

3024 reflections with $I > 2\sigma(I)$

$R_{int} = 0.064$

$\theta_{max} = 38.5°$, $\theta_{min} = 3.1°$

$h = -15 \rightarrow 16$

$k = -17 \rightarrow 17$

$l = -15 \rightarrow 22$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.050$

$wR(F^2) = 0.147$

$S = 1.08$

3594 reflections

217 parameters

0 restraints

Primary atom site location: difference Fourier
    map

Secondary atom site location: difference Fourier
    map

Hydrogen site location: mixed

H atoms treated by a mixture of independent
    and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0669P)^2 + 2.4P]$
    where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.71$ e Å^{-3}

$\Delta\rho_{min} = -0.72$ 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 (Å^2)

	x	y	z	$U_{iso}*/U_{eq}$
S1	0.02475 (4)	0.39698 (3)	0.79544 (3)	0.02956 (19)
O1	0.22041 (10)	0.74793 (9)	0.57892 (8)	0.0307 (3)
N1	0.25131 (12)	0.45803 (11)	0.55151 (9)	0.0249 (4)
H1	0.2524 (17)	0.3954 (19)	0.5496 (12)	0.030*
C2	0.26696 (14)	0.49600 (12)	0.62814 (11)	0.0244 (4)
H2	0.3287	0.4706	0.6463	0.029*
N3	0.27450 (11)	0.60304 (10)	0.62410 (9)	0.0229 (4)
C4	0.22059 (13)	0.65770 (13)	0.57606 (10)	0.0231 (4)
C4A	0.16533 (14)	0.60308 (12)	0.51890 (10)	0.0228 (4)
C5	0.10052 (15)	0.65191 (14)	0.47233 (11)	0.0276 (4)
H5	0.0882	0.7184	0.4810	0.033*
C6	0.05414 (17)	0.60404 (15)	0.41351 (12)	0.0333 (5)
H6	0.0103	0.6371	0.3823	0.040*
C7	0.07389 (16)	0.50578 (16)	0.40152 (12)	0.0336 (5)
H7	0.0433	0.4727	0.3613	0.040*
C8	0.13683 (15)	0.45601 (14)	0.44685 (11)	0.0301 (5)

H8	0.1487	0.3896	0.4376	0.036*
C8A	0.18367 (13)	0.50393 (12)	0.50701 (10)	0.0234 (4)
C9	0.19299 (14)	0.46488 (12)	0.68451 (11)	0.0244 (4)
H9	0.1295	0.4819	0.6749	0.029*
C10	0.21254 (15)	0.41433 (13)	0.74758 (11)	0.0264 (4)
H10	0.2767	0.3995	0.7566	0.032*
C11	0.14428 (15)	0.37959 (13)	0.80424 (10)	0.0256 (4)
C12	0.16756 (16)	0.32822 (13)	0.87251 (11)	0.0304 (3)
H12	0.2292	0.3110	0.8879	0.037*
C13	0.08295 (16)	0.30680 (14)	0.91398 (11)	0.0304 (3)
H13	0.0830	0.2734	0.9610	0.037*
C14	0.00234 (17)	0.33875 (14)	0.87974 (11)	0.0304 (3)
H14	−0.0588	0.3298	0.9002	0.037*
C15	0.33187 (14)	0.64888 (13)	0.68295 (11)	0.0265 (4)
H15A	0.3163	0.6195	0.7326	0.032*
H15B	0.3156	0.7183	0.6856	0.032*
C16	0.43773 (14)	0.63919 (12)	0.66925 (10)	0.0224 (4)
C17	0.47531 (15)	0.60700 (13)	0.60001 (11)	0.0261 (4)
H17	0.4345	0.5901	0.5595	0.031*
C18	0.57301 (16)	0.59978 (14)	0.59048 (12)	0.0313 (5)
H18	0.5982	0.5765	0.5441	0.038*
C19	0.63326 (16)	0.62705 (15)	0.64953 (13)	0.0345 (5)
H19	0.6993	0.6232	0.6429	0.041*
C20	0.59602 (16)	0.66002 (14)	0.71824 (13)	0.0330 (5)
H20	0.6368	0.6793	0.7581	0.040*
C21	0.49895 (15)	0.66462 (13)	0.72819 (11)	0.0257 (4)
H21	0.4741	0.6852	0.7755	0.031*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0350 (4)	0.0244 (3)	0.0293 (3)	0.00022 (19)	0.0016 (2)	0.00190 (17)
O1	0.0362 (9)	0.0153 (6)	0.0407 (8)	−0.0011 (6)	−0.0010 (6)	−0.0009 (5)
N1	0.0316 (10)	0.0150 (7)	0.0280 (8)	0.0016 (6)	0.0027 (7)	−0.0011 (6)
C2	0.0263 (11)	0.0178 (8)	0.0292 (9)	0.0015 (7)	0.0010 (8)	0.0008 (7)
N3	0.0224 (9)	0.0165 (7)	0.0298 (8)	−0.0006 (6)	−0.0011 (7)	−0.0017 (6)
C4	0.0232 (10)	0.0177 (8)	0.0284 (9)	0.0001 (7)	0.0038 (7)	0.0004 (6)
C4A	0.0245 (11)	0.0186 (8)	0.0253 (9)	−0.0016 (7)	0.0043 (8)	0.0010 (6)
C5	0.0306 (11)	0.0236 (8)	0.0285 (9)	0.0014 (8)	0.0029 (8)	0.0012 (7)
C6	0.0345 (13)	0.0369 (11)	0.0286 (10)	0.0016 (9)	−0.0012 (9)	0.0013 (8)
C7	0.0358 (12)	0.0365 (11)	0.0287 (10)	−0.0053 (9)	−0.0014 (9)	−0.0059 (8)
C8	0.0363 (12)	0.0237 (9)	0.0305 (10)	−0.0043 (8)	0.0063 (8)	−0.0050 (7)
C8A	0.0249 (10)	0.0203 (8)	0.0250 (9)	−0.0031 (7)	0.0058 (7)	0.0005 (7)
C9	0.0237 (10)	0.0201 (8)	0.0295 (9)	0.0012 (7)	0.0022 (8)	−0.0011 (7)
C10	0.0291 (11)	0.0213 (8)	0.0288 (9)	0.0005 (7)	−0.0004 (8)	−0.0020 (7)
C11	0.0325 (12)	0.0194 (8)	0.0248 (9)	0.0009 (8)	−0.0008 (8)	−0.0018 (7)
C12	0.0409 (7)	0.0244 (5)	0.0260 (5)	0.0018 (5)	0.0042 (5)	−0.0015 (4)
C13	0.0409 (7)	0.0244 (5)	0.0260 (5)	0.0018 (5)	0.0042 (5)	−0.0015 (4)

C14	0.0409 (7)	0.0244 (5)	0.0260 (5)	0.0018 (5)	0.0042 (5)	−0.0015 (4)
C15	0.0272 (11)	0.0240 (8)	0.0283 (9)	0.0007 (8)	0.0004 (8)	−0.0044 (7)
C16	0.0239 (10)	0.0173 (8)	0.0260 (9)	−0.0003 (7)	−0.0001 (7)	0.0028 (6)
C17	0.0282 (12)	0.0220 (9)	0.0281 (10)	−0.0006 (7)	0.0025 (8)	0.0037 (7)
C18	0.0339 (12)	0.0258 (9)	0.0341 (10)	0.0020 (8)	0.0087 (9)	0.0066 (7)
C19	0.0259 (11)	0.0284 (9)	0.0492 (12)	0.0014 (8)	0.0031 (10)	0.0107 (9)
C20	0.0327 (13)	0.0254 (9)	0.0409 (11)	−0.0002 (8)	−0.0079 (9)	0.0048 (8)
C21	0.0279 (11)	0.0194 (8)	0.0297 (9)	0.0011 (8)	−0.0022 (8)	0.0021 (7)

Geometric parameters (Å, º)

S1—C14	1.721 (2)	C9—H9	0.9500
S1—C11	1.727 (2)	C10—C11	1.475 (3)
O1—C4	1.251 (2)	C10—H10	0.9500
N1—C8A	1.396 (3)	C11—C12	1.437 (3)
N1—C2	1.467 (2)	C12—C13	1.440 (3)
N1—H1	0.87 (3)	C12—H12	0.9500
C2—N3	1.489 (2)	C13—C14	1.371 (3)
C2—C9	1.511 (3)	C13—H13	0.9500
C2—H2	1.0000	C14—H14	0.9500
N3—C4	1.371 (2)	C15—C16	1.533 (3)
N3—C15	1.465 (2)	C15—H15A	0.9900
C4—C4A	1.486 (3)	C15—H15B	0.9900
C4A—C5	1.409 (3)	C16—C21	1.402 (3)
C4A—C8A	1.414 (2)	C16—C17	1.406 (3)
C5—C6	1.397 (3)	C17—C18	1.405 (3)
C5—H5	0.9500	C17—H17	0.9500
C6—C7	1.406 (3)	C18—C19	1.401 (3)
C6—H6	0.9500	C18—H18	0.9500
C7—C8	1.385 (3)	C19—C20	1.399 (3)
C7—H7	0.9500	C19—H19	0.9500
C8—C8A	1.418 (3)	C20—C21	1.395 (3)
C8—H8	0.9500	C20—H20	0.9500
C9—C10	1.343 (3)	C21—H21	0.9500
C14—S1—C11	92.28 (10)	C9—C10—H10	116.8
C8A—N1—C2	117.34 (15)	C11—C10—H10	116.8
C8A—N1—H1	116.5 (16)	C12—C11—C10	125.22 (19)
C2—N1—H1	113.1 (15)	C12—C11—S1	111.83 (15)
N1—C2—N3	108.92 (14)	C10—C11—S1	122.94 (14)
N1—C2—C9	113.41 (16)	C11—C12—C13	109.51 (19)
N3—C2—C9	111.47 (15)	C11—C12—H12	125.2
N1—C2—H2	107.6	C13—C12—H12	125.2
N3—C2—H2	107.6	C14—C13—C12	114.26 (18)
C9—C2—H2	107.6	C14—C13—H13	122.9
C4—N3—C15	120.68 (15)	C12—C13—H13	122.9
C4—N3—C2	122.63 (15)	C13—C14—S1	112.11 (17)
C15—N3—C2	115.99 (15)	C13—C14—H14	123.9

O1—C4—N3	121.87 (17)	S1—C14—H14	123.9
O1—C4—C4A	122.35 (17)	N3—C15—C16	113.52 (15)
N3—C4—C4A	115.74 (15)	N3—C15—H15A	108.9
C5—C4A—C8A	120.09 (17)	C16—C15—H15A	108.9
C5—C4A—C4	119.86 (16)	N3—C15—H15B	108.9
C8A—C4A—C4	119.83 (17)	C16—C15—H15B	108.9
C6—C5—C4A	120.97 (18)	H15A—C15—H15B	107.7
C6—C5—H5	119.5	C21—C16—C17	119.12 (18)
C4A—C5—H5	119.5	C21—C16—C15	118.25 (17)
C5—C6—C7	118.5 (2)	C17—C16—C15	122.63 (17)
C5—C6—H6	120.8	C18—C17—C16	120.24 (19)
C7—C6—H6	120.8	C18—C17—H17	119.9
C8—C7—C6	121.66 (19)	C16—C17—H17	119.9
C8—C7—H7	119.2	C19—C18—C17	119.90 (19)
C6—C7—H7	119.2	C19—C18—H18	120.0
C7—C8—C8A	120.21 (18)	C17—C18—H18	120.0
C7—C8—H8	119.9	C20—C19—C18	119.9 (2)
C8A—C8—H8	119.9	C20—C19—H19	120.0
N1—C8A—C4A	119.13 (17)	C18—C19—H19	120.0
N1—C8A—C8	122.14 (16)	C21—C20—C19	120.0 (2)
C4A—C8A—C8	118.60 (17)	C21—C20—H20	120.0
C10—C9—C2	123.27 (19)	C19—C20—H20	120.0
C10—C9—H9	118.4	C20—C21—C16	120.79 (19)
C2—C9—H9	118.4	C20—C21—H21	119.6
C9—C10—C11	126.45 (19)	C16—C21—H21	119.6
C8A—N1—C2—N3	−46.4 (2)	C7—C8—C8A—C4A	−0.6 (3)
C8A—N1—C2—C9	78.4 (2)	N1—C2—C9—C10	120.5 (2)
N1—C2—N3—C4	37.7 (2)	N3—C2—C9—C10	−116.17 (19)
C9—C2—N3—C4	−88.2 (2)	C2—C9—C10—C11	−178.56 (17)
N1—C2—N3—C15	−151.91 (16)	C9—C10—C11—C12	−177.92 (18)
C9—C2—N3—C15	82.2 (2)	C9—C10—C11—S1	2.0 (3)
C15—N3—C4—O1	2.2 (3)	C14—S1—C11—C12	0.19 (15)
C2—N3—C4—O1	172.24 (17)	C14—S1—C11—C10	−179.70 (16)
C15—N3—C4—C4A	−179.85 (16)	C10—C11—C12—C13	179.56 (17)
C2—N3—C4—C4A	−9.9 (3)	S1—C11—C12—C13	−0.3 (2)
O1—C4—C4A—C5	−8.7 (3)	C11—C12—C13—C14	0.4 (2)
N3—C4—C4A—C5	173.42 (17)	C12—C13—C14—S1	−0.2 (2)
O1—C4—C4A—C8A	165.94 (18)	C11—S1—C14—C13	0.02 (16)
N3—C4—C4A—C8A	−11.9 (3)	C4—N3—C15—C16	−112.23 (18)
C8A—C4A—C5—C6	−0.6 (3)	C2—N3—C15—C16	77.1 (2)
C4—C4A—C5—C6	174.00 (18)	N3—C15—C16—C21	−168.65 (15)
C4A—C5—C6—C7	−0.3 (3)	N3—C15—C16—C17	12.1 (2)
C5—C6—C7—C8	0.7 (3)	C21—C16—C17—C18	0.5 (3)
C6—C7—C8—C8A	−0.3 (3)	C15—C16—C17—C18	179.79 (16)
C2—N1—C8A—C4A	28.7 (2)	C16—C17—C18—C19	−1.6 (3)
C2—N1—C8A—C8	−155.42 (18)	C17—C18—C19—C20	1.0 (3)
C5—C4A—C8A—N1	177.06 (17)	C18—C19—C20—C21	0.8 (3)

C4—C4A—C8A—N1	2.4 (3)	C19—C20—C21—C16	−1.9 (3)
C5—C4A—C8A—C8	1.1 (3)	C17—C16—C21—C20	1.2 (3)
C4—C4A—C8A—C8	−173.56 (17)	C15—C16—C21—C20	−178.09 (17)
C7—C8—C8A—N1	−176.50 (18)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1[i]	0.87 (3)	2.14 (3)	2.978 (2)	161 (2)

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