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3-*tert*-Butyl-4-(4-chlorophenyl)-1-phenyl-1*H*-pyrazolo[3,4-e][1,4]thiazepin-7(4*H*,6*H*,8*H*)-one

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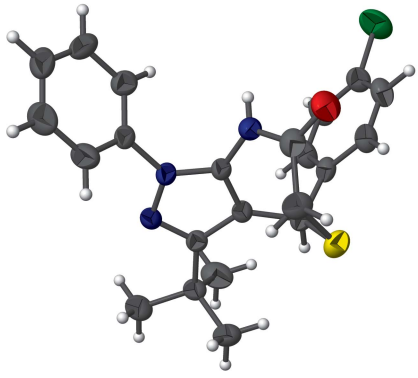
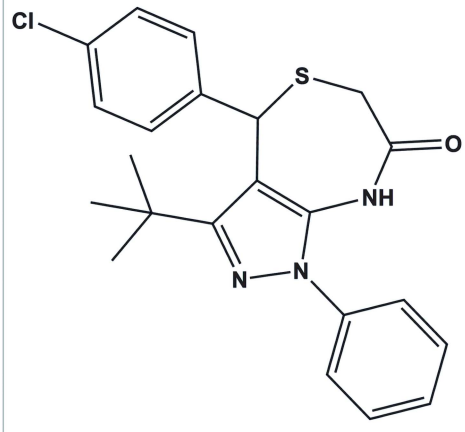
In the title molecule, $C_{22}H_{22}ClN_3OS$, the fused 1,4-thiazepinone ring adopts a near twist-boat conformation and the chlorobenzene ring is inclined to the phenyl ring by 88.38 (12)°. In the crystal, molecules are linked by pairs of N—H···O hydrogen bonds, forming inversion dimers with an $R_2^2(8)$ ring motif. The dimers are linked *via* C—H···O hydrogen bonds forming ribbons, enclosing $R_4^2(20)$ loops, propagating along [001].

3D view



Chemical scheme



Structure description

The title compound has in its structure the 1,4-thiazepine ring which is one of the most important moieties in nitrogen- and sulfur-containing heterocycles and which has been widely used as a building block for pharmacologically relevant therapeutic agents. Nowadays, the design of 1,4-thiazepines fused with bioactive heteroaromatic scaffolds is highly valuable for medicinal chemistry and drug discovery (Chen & Shi, 2011).

A perspective view of the title compound, with a folded structure, showing the atomic numbering scheme, is given in Fig. 1. From the puckering analysis [$q2$ = 1.076 (2) Å, $\varphi3$ = −106.3 (7)°, $q3$ = 0.211 (2) Å and $\varphi2$ = −167.2 (1)°], the fused 1,4-thiazepinone ring (S1/C9/C8/N3/C7/C17/C10) adopts a near twist-boat conformation. The benzene (C11–C16) and phenyl (C1–C6) rings are normal to one another, with a dihedral anble of 88.38 (12)°.

In the crystal, molecules are linked by pairs of N—H···O hydrogen bonds, of moderate strength (Desiraju & Steiner, 1999), forming inversion dimers enclosing an $R_2^2(8)$ ring motif (Table 1 and Fig. 2). The dimers are linked *via* C—H···O hydrogen bonds forming ribbons, enclosing $R_4^2(20)$ loops, propagating along the *c*-axis direction (Table 1 and Fig. 2).

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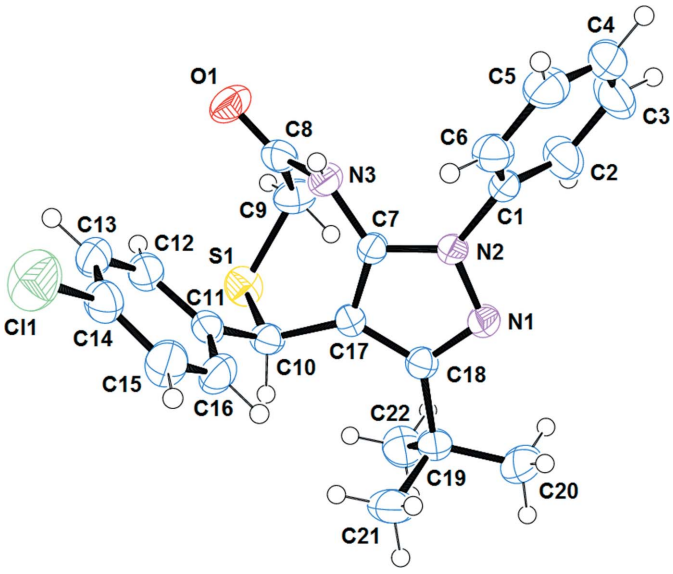

Figure 1
The molecular structure of the title compound, with atom labelling and displacement ellipsoids drawn at the 50% probability level.

Synthesis and crystallization

A 5 ml pyrex test tube was charged with a mixture of 3-(*tert*-butyl)-1-phenyl-1*H*-pyrazol-5-amine (111 mg, 0.52 mmol), *p*-chlorobenzaldehyde (73 mg, 0.52 mmol) and 2-mercaptoacetic acid (57 mg, 0.62 mmol) in the absence of solvent. The mixture was heated in an oil bath at 393 K for 20 min until the starting materials were no longer detected by thin-layer chromatography. Then, the obtained oily material was purified by column chromatography on silica gel using a mixture of CH_2Cl_2/EtOAc (10:1) as eluent. Yellow crystals suitable for single-crystal X-ray diffraction were grown by slow evaporation, at ambient temperature and in air, from a solution in methanol [81% yield, m.p. 518 (1) K].

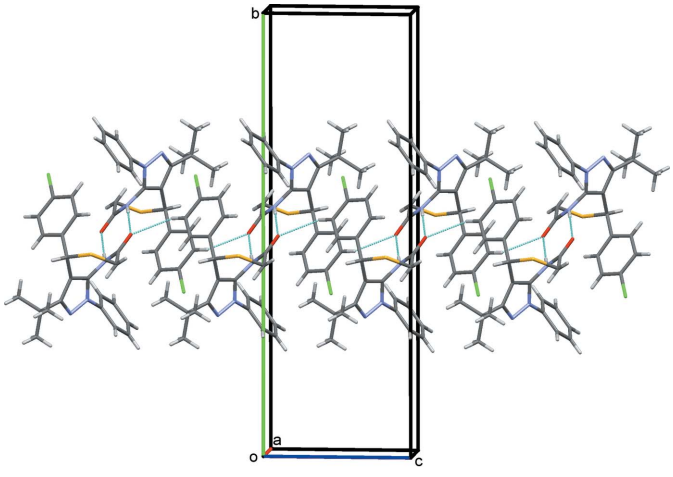

Figure 2
A partial view along the *a* axis of the crystal packing of the title compound, with hydrogen bonds shown as dashed lines (see Table 1).

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H31···O1^{i}	0.81 (2)	2.10 (2)	2.897 (3)	170 (2)
C15—H15···O1^{ii}	0.93	2.56	3.372 (3)	146

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{22}H_{22}ClN_3OS$
M_r	411.94
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	295
a, b, c (Å)	9.7478 (3), 25.2229 (8), 8.6354 (2)
β (°)	101.733 (2)
V (Å^3)	2078.80 (10)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.30
Crystal size (mm)	0.46 × 0.45 × 0.20
Data collection	
Diffractometer	Oxford Diffraction Gemini S
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	4362, 4251, 2417
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.048, 0.115, 0.95
No. of reflections	4251
No. of parameters	257
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.40, −0.38

Computer programs: *COLLECT* (Nonius, 2000), *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997, *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2006).

Refinement

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

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x160608 [doi:10.1107/S2414314616006088]

3-*tert*-Butyl-4-(4-chlorophenyl)-1-phenyl-1*H*-pyrazolo[3,4-*e*][1,4]thiazepin-7(4*H*,6*H*,8*H*)-one

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(I)

Crystal data

$C_{22}H_{22}ClN_3OS$
M_r = 411.94
Monoclinic, $P2_1/c$
a = 9.7478 (3) Å
b = 25.2229 (8) Å
c = 8.6354 (2) Å
β = 101.733 (2)°
V = 2078.80 (10) Å^3
Z = 4
$F(000)$ = 864
D_x = 1.313 Mg m^{-3}
Melting point: 518(1) K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7625 reflections
θ = 3.2–26.4°
μ = 0.30 mm^{-1}
T = 295 K
Block, yellow
0.46 × 0.45 × 0.20 mm

Data collection

Oxford Diffraction Gemini S diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
4362 measured reflections
4251 independent reflections
2417 reflections with $I > 2\sigma(I)$
R_{int} = 0
θ_{max} = 26.4°, θ_{min} = 3.2°
h = 0→12
k = −31→0
l = −10→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.115
S = 0.95
4251 reflections
257 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0442P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Special details

Experimental. IR spectra was recorded on a FT—IR SHIMADZU IR-Affinity-1 spectrophotometer. IR (KBr): cm^{-1}, 3424 (N-H), 2972, 2929, 1686 (C=O). MS (IE, 70 eV) m/z (%): 413/411 (16/47) [M+], 366/364 (5/15), 300 (100), 226 (7), 77 (16).

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.

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}
S1	0.45801 (6)	0.54058 (3)	0.14582 (7)	0.0460 (2)
Cl1	0.00759 (8)	0.36932 (3)	0.45897 (8)	0.0741 (3)
O1	0.13987 (16)	0.50033 (7)	−0.10709 (18)	0.0515 (5)
N1	0.18428 (17)	0.67941 (8)	0.30062 (19)	0.0346 (5)
N2	0.10134 (17)	0.64849 (8)	0.18983 (19)	0.0338 (5)
N3	0.1012 (2)	0.56179 (8)	0.0695 (2)	0.0357 (5)
C1	−0.0292 (2)	0.66867 (10)	0.1018 (2)	0.0347 (6)
C2	−0.0295 (3)	0.71213 (11)	0.0076 (3)	0.0582 (8)
H2	0.0543	0.7287	0.0005	0.070*
C3	−0.1555 (3)	0.73149 (12)	−0.0774 (4)	0.0743 (9)
H3	−0.1567	0.7611	−0.1419	0.089*
C4	−0.2783 (3)	0.70688 (12)	−0.0661 (3)	0.0663 (9)
H4	−0.3630	0.7200	−0.1227	0.080*
C5	−0.2771 (2)	0.66330 (12)	0.0276 (3)	0.0550 (8)
H5	−0.3609	0.6467	0.0344	0.066*
C6	−0.1519 (2)	0.64363 (10)	0.1128 (3)	0.0442 (6)
H6	−0.1508	0.6139	0.1766	0.053*
C7	0.1570 (2)	0.59975 (9)	0.1837 (2)	0.0310 (5)
C8	0.1808 (2)	0.53877 (11)	−0.0234 (2)	0.0402 (6)
C9	0.3205 (2)	0.56410 (10)	−0.0200 (2)	0.0455 (7)
H91	0.3795	0.5507	−0.0827	0.055*
H92	0.3482	0.5932	0.0449	0.055*
C10	0.3714 (2)	0.54898 (10)	0.3150 (2)	0.0363 (6)
H101	0.4456	0.5554	0.4082	0.044*
C11	0.2902 (2)	0.50020 (9)	0.3514 (2)	0.0347 (6)
C12	0.2652 (2)	0.45570 (10)	0.2574 (2)	0.0416 (6)
H12	0.3067	0.4528	0.1698	0.050*
C13	0.1798 (2)	0.41520 (10)	0.2907 (3)	0.0449 (6)
H13	0.1627	0.3857	0.2250	0.054*
C14	0.1208 (2)	0.41892 (10)	0.4204 (3)	0.0449 (6)
C15	0.1480 (3)	0.46167 (11)	0.5211 (3)	0.0521 (7)
H15	0.1105	0.4633	0.6118	0.063*
C16	0.2314 (3)	0.50199 (10)	0.4854 (3)	0.0479 (7)
H16	0.2490	0.5311	0.5524	0.057*
C17	0.2802 (2)	0.59764 (9)	0.2920 (2)	0.0311 (5)
C18	0.2939 (2)	0.64881 (9)	0.3612 (2)	0.0322 (5)

C19	0.4095 (2)	0.67068 (10)	0.4904 (2)	0.0389 (6)
C20	0.3832 (3)	0.72886 (10)	0.5220 (3)	0.0578 (8)
H201	0.4572	0.7419	0.6039	0.087*
H202	0.3805	0.7490	0.4271	0.087*
H203	0.2953	0.7323	0.5549	0.087*
C21	0.4139 (3)	0.63899 (11)	0.6429 (3)	0.0607 (8)
H211	0.4868	0.6527	0.7250	0.091*
H212	0.3254	0.6421	0.6747	0.091*
H213	0.4321	0.6024	0.6246	0.091*
C22	0.5510 (2)	0.66588 (11)	0.4380 (3)	0.0549 (7)
H221	0.6243	0.6797	0.5194	0.082*
H222	0.5694	0.6293	0.4195	0.082*
H223	0.5474	0.6857	0.3423	0.082*
H31	0.029 (2)	0.5480 (9)	0.080 (2)	0.029 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0383 (3)	0.0523 (5)	0.0503 (4)	0.0067 (3)	0.0156 (3)	0.0009 (3)
Cl1	0.0895 (6)	0.0602 (6)	0.0791 (5)	−0.0211 (4)	0.0326 (4)	0.0031 (4)
O1	0.0585 (11)	0.0504 (13)	0.0452 (9)	−0.0022 (9)	0.0098 (8)	−0.0194 (9)
N1	0.0331 (10)	0.0306 (12)	0.0381 (10)	−0.0008 (9)	0.0020 (8)	−0.0035 (9)
N2	0.0298 (10)	0.0320 (13)	0.0357 (10)	0.0047 (9)	−0.0022 (8)	−0.0062 (9)
N3	0.0321 (11)	0.0355 (13)	0.0383 (11)	0.0000 (10)	0.0044 (9)	−0.0080 (10)
C1	0.0336 (13)	0.0321 (15)	0.0354 (12)	0.0047 (11)	−0.0001 (10)	−0.0082 (11)
C2	0.0475 (16)	0.0399 (19)	0.0778 (18)	−0.0054 (13)	−0.0097 (14)	0.0099 (15)
C3	0.068 (2)	0.043 (2)	0.095 (2)	0.0040 (16)	−0.0237 (17)	0.0180 (16)
C4	0.0500 (18)	0.050 (2)	0.084 (2)	0.0145 (15)	−0.0217 (15)	−0.0162 (18)
C5	0.0325 (14)	0.066 (2)	0.0627 (16)	0.0041 (14)	0.0009 (12)	−0.0188 (16)
C6	0.0402 (14)	0.0478 (18)	0.0427 (13)	−0.0001 (13)	0.0043 (11)	−0.0038 (12)
C7	0.0301 (12)	0.0286 (15)	0.0331 (12)	0.0019 (11)	0.0039 (10)	−0.0047 (11)
C8	0.0455 (14)	0.0437 (17)	0.0297 (12)	0.0056 (13)	0.0038 (11)	0.0021 (13)
C9	0.0425 (14)	0.0595 (19)	0.0368 (13)	−0.0027 (13)	0.0130 (11)	−0.0078 (12)
C10	0.0339 (12)	0.0406 (16)	0.0324 (12)	0.0047 (11)	0.0020 (9)	−0.0018 (11)
C11	0.0374 (13)	0.0354 (16)	0.0305 (12)	0.0094 (11)	0.0051 (10)	0.0019 (11)
C12	0.0531 (15)	0.0390 (17)	0.0345 (12)	0.0072 (13)	0.0134 (11)	0.0007 (12)
C13	0.0620 (16)	0.0349 (17)	0.0379 (13)	0.0033 (13)	0.0105 (12)	−0.0032 (12)
C14	0.0491 (14)	0.0391 (17)	0.0465 (14)	−0.0018 (13)	0.0098 (12)	0.0067 (13)
C15	0.0767 (18)	0.0451 (19)	0.0406 (14)	−0.0013 (15)	0.0262 (13)	0.0020 (14)
C16	0.0697 (17)	0.0371 (17)	0.0384 (13)	−0.0002 (14)	0.0145 (12)	−0.0074 (12)
C17	0.0316 (12)	0.0292 (15)	0.0318 (11)	0.0017 (11)	0.0049 (10)	0.0015 (11)
C18	0.0318 (12)	0.0328 (15)	0.0318 (11)	0.0002 (11)	0.0058 (9)	0.0000 (11)
C19	0.0356 (13)	0.0371 (16)	0.0394 (12)	−0.0018 (11)	−0.0031 (10)	−0.0034 (12)
C20	0.0535 (16)	0.051 (2)	0.0612 (16)	−0.0043 (14)	−0.0062 (13)	−0.0178 (14)
C21	0.0670 (17)	0.066 (2)	0.0409 (14)	−0.0129 (15)	−0.0092 (12)	0.0001 (14)
C22	0.0379 (14)	0.053 (2)	0.0690 (17)	−0.0065 (13)	0.0006 (12)	−0.0006 (15)

Geometric parameters (Å, º)

S1—C10	1.842 (2)	C10—C11	1.530 (3)
S1—C9	1.849 (2)	C10—H101	0.9800
Cl1—C14	1.745 (2)	C11—C12	1.378 (3)
O1—C8	1.226 (3)	C11—C16	1.392 (3)
N1—C18	1.336 (3)	C12—C13	1.385 (3)
N1—N2	1.365 (2)	C12—H12	0.9300
N2—C7	1.349 (3)	C13—C14	1.362 (3)
N2—C1	1.436 (2)	C13—H13	0.9300
N3—C8	1.355 (3)	C14—C15	1.377 (3)
N3—C7	1.402 (3)	C15—C16	1.376 (3)
N3—H31	0.81 (2)	C15—H15	0.9300
C1—C2	1.365 (3)	C16—H16	0.9300
C1—C6	1.373 (3)	C17—C18	1.417 (3)
C2—C3	1.385 (3)	C18—C19	1.519 (3)
C2—H2	0.9300	C19—C20	1.524 (3)
C3—C4	1.369 (4)	C19—C21	1.534 (3)
C3—H3	0.9300	C19—C22	1.541 (3)
C4—C5	1.364 (4)	C20—H201	0.9600
C4—H4	0.9300	C20—H202	0.9600
C5—C6	1.383 (3)	C20—H203	0.9600
C5—H5	0.9300	C21—H211	0.9600
C6—H6	0.9300	C21—H212	0.9600
C7—C17	1.365 (3)	C21—H213	0.9600
C8—C9	1.499 (3)	C22—H221	0.9600
C9—H91	0.9300	C22—H222	0.9600
C9—H92	0.9300	C22—H223	0.9600
C10—C17	1.505 (3)		
C10—S1—C9	101.56 (10)	C16—C11—C10	117.6 (2)
C18—N1—N2	104.91 (17)	C11—C12—C13	121.3 (2)
C7—N2—N1	111.25 (16)	C11—C12—H12	119.3
C7—N2—C1	128.48 (17)	C13—C12—H12	119.3
N1—N2—C1	120.23 (18)	C14—C13—C12	119.5 (2)
C8—N3—C7	121.5 (2)	C14—C13—H13	120.3
C8—N3—H31	119.9 (15)	C12—C13—H13	120.3
C7—N3—H31	116.1 (15)	C13—C14—C15	121.0 (2)
C2—C1—C6	121.0 (2)	C13—C14—Cl1	119.8 (2)
C2—C1—N2	119.7 (2)	C15—C14—Cl1	119.25 (19)
C6—C1—N2	119.4 (2)	C16—C15—C14	118.9 (2)
C1—C2—C3	119.6 (2)	C16—C15—H15	120.5
C1—C2—H2	120.2	C14—C15—H15	120.5
C3—C2—H2	120.2	C15—C16—C11	121.6 (2)
C4—C3—C2	119.7 (3)	C15—C16—H16	119.2
C4—C3—H3	120.1	C11—C16—H16	119.2
C2—C3—H3	120.1	C7—C17—C18	104.37 (18)
C5—C4—C3	120.4 (2)	C7—C17—C10	122.4 (2)

C5—C4—H4	119.8	C18—C17—C10	133.19 (18)
C3—C4—H4	119.8	N1—C18—C17	111.19 (17)
C4—C5—C6	120.3 (3)	N1—C18—C19	119.5 (2)
C4—C5—H5	119.8	C17—C18—C19	129.26 (19)
C6—C5—H5	119.8	C18—C19—C20	110.76 (18)
C1—C6—C5	119.0 (2)	C18—C19—C21	109.17 (19)
C1—C6—H6	120.5	C20—C19—C21	108.9 (2)
C5—C6—H6	120.5	C18—C19—C22	109.26 (18)
N2—C7—C17	108.26 (18)	C20—C19—C22	108.7 (2)
N2—C7—N3	123.23 (17)	C21—C19—C22	109.96 (19)
C17—C7—N3	128.1 (2)	C19—C20—H201	109.5
O1—C8—N3	122.1 (2)	C19—C20—H202	109.5
O1—C8—C9	122.3 (2)	H201—C20—H202	109.5
N3—C8—C9	115.6 (2)	C19—C20—H203	109.5
C8—C9—S1	113.04 (16)	H201—C20—H203	109.5
C8—C9—H91	120.0	H202—C20—H203	109.5
S1—C9—H91	84.1	C19—C21—H211	109.5
C8—C9—H92	120.0	C19—C21—H212	109.5
S1—C9—H92	73.2	H211—C21—H212	109.5
H91—C9—H92	120.0	C19—C21—H213	109.5
C17—C10—C11	111.46 (17)	H211—C21—H213	109.5
C17—C10—S1	110.06 (14)	H212—C21—H213	109.5
C11—C10—S1	114.23 (15)	C19—C22—H221	109.5
C17—C10—H101	106.9	C19—C22—H222	109.5
C11—C10—H101	106.9	H221—C22—H222	109.5
S1—C10—H101	106.9	C19—C22—H223	109.5
C12—C11—C16	117.6 (2)	H221—C22—H223	109.5
C12—C11—C10	124.8 (2)	H222—C22—H223	109.5

C18—N1—N2—C7	0.9 (2)	C16—C11—C12—C13	2.8 (3)
C18—N1—N2—C1	178.85 (19)	C10—C11—C12—C13	−173.9 (2)
C7—N2—C1—C2	−121.2 (3)	C11—C12—C13—C14	−1.1 (3)
N1—N2—C1—C2	61.2 (3)	C12—C13—C14—C15	−1.7 (3)
C7—N2—C1—C6	58.3 (3)	C12—C13—C14—Cl1	177.52 (18)
N1—N2—C1—C6	−119.2 (2)	C13—C14—C15—C16	2.7 (4)
C6—C1—C2—C3	0.4 (4)	Cl1—C14—C15—C16	−176.60 (18)
N2—C1—C2—C3	179.9 (2)	C14—C15—C16—C11	−0.8 (4)
C1—C2—C3—C4	0.0 (4)	C12—C11—C16—C15	−1.9 (3)
C2—C3—C4—C5	−0.3 (4)	C10—C11—C16—C15	175.1 (2)
C3—C4—C5—C6	0.3 (4)	N2—C7—C17—C18	−0.7 (2)
C2—C1—C6—C5	−0.5 (3)	N3—C7—C17—C18	172.0 (2)
N2—C1—C6—C5	179.99 (19)	N2—C7—C17—C10	−179.07 (19)
C4—C5—C6—C1	0.2 (4)	N3—C7—C17—C10	−6.4 (3)
N1—N2—C7—C17	−0.2 (2)	C11—C10—C17—C7	−55.6 (3)
C1—N2—C7—C17	−177.8 (2)	S1—C10—C17—C7	72.2 (2)
N1—N2—C7—N3	−173.25 (19)	C11—C10—C17—C18	126.5 (2)
C1—N2—C7—N3	9.1 (3)	S1—C10—C17—C18	−105.7 (2)
C8—N3—C7—N2	125.2 (2)	N2—N1—C18—C17	−1.4 (2)

C8—N3—C7—C17	−46.5 (3)	N2—N1—C18—C19	−179.90 (18)
C7—N3—C8—O1	169.2 (2)	C7—C17—C18—N1	1.3 (2)
C7—N3—C8—C9	−12.1 (3)	C10—C17—C18—N1	179.5 (2)
O1—C8—C9—S1	−96.7 (2)	C7—C17—C18—C19	179.6 (2)
N3—C8—C9—S1	84.6 (2)	C10—C17—C18—C19	−2.2 (4)
C10—S1—C9—C8	−50.4 (2)	N1—C18—C19—C20	−4.3 (3)
C9—S1—C10—C17	−35.57 (17)	C17—C18—C19—C20	177.5 (2)
C9—S1—C10—C11	90.69 (16)	N1—C18—C19—C21	115.6 (2)
C17—C10—C11—C12	117.2 (2)	C17—C18—C19—C21	−62.6 (3)
S1—C10—C11—C12	−8.3 (3)	N1—C18—C19—C22	−124.1 (2)
C17—C10—C11—C16	−59.6 (2)	C17—C18—C19—C22	57.7 (3)
S1—C10—C11—C16	174.91 (15)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H31···O1^{i}	0.81 (2)	2.10 (2)	2.897 (3)	170 (2)
C15—H15···O1^{ii}	0.93	2.56	3.372 (3)	146

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