Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(2*R*)-*N*-[5-(4-Chlorophenyl)-1,3,4-thiadiazol-2-yl]-2-(cinnamoylamino)-propanamide

Shao-Hua Li,[a,b] Hui-Ming Huang,[b] Bin-Hai Kuang,[b] Guo-Gang Tu[b]* and Cheng-Mei Liu[a]‡

[a]State Key Laboratory of Food Science and Technology, Nanchang University, 330047 Nanchang, JiangXi, People's Republic of China, and [b]Department of Pharmacy, NanChang University Medical College, 330006 Nanchang, JiangXi, People's Republic of China
Correspondence e-mail: tugg199@yahoo.com

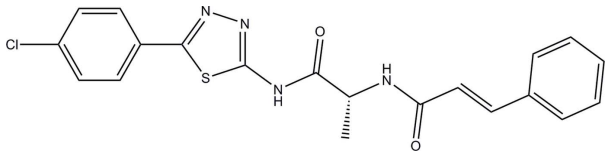
Received 5 September 2008; accepted 22 September 2008

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.043; wR factor = 0.099; data-to-parameter ratio = 18.5.

In the title compound, $C_{20}H_{17}ClN_4O_2S$, the dihedral angle between the two benzene rings is 65.9 (1)°; the corresponding angle between the 4-chlorophenyl and thiadiazole rings is 3.4 (8)°. The conformations of the N—H and C═O bonds are *anti* with respect to each other. The enone groups show a *trans* configuration. The structure displays intermolecular N—H···O, C—H···N, C—H···S and C—H···O hydrogen bonding.

Related literature

For 1,3,4-thiadiazole scaffold compounds and their biological activity, see: Tu *et al.* (2008). For the synthesis, see: Foroumadi *et al.* (1999); Levy & Palmer (1942); Song *et al.* (1992). For related structures, see: Fun *et al.* (2008); Gowda *et al.* (2008) Thiruvalluvar *et al.* (2008).



Experimental

Crystal data

$C_{20}H_{17}ClN_4O_2S$
M_r = 412.89
Orthorhombic, $P2_12_12_1$
a = 6.6324 (15) Å
b = 8.575 (2) Å
c = 34.367 (8) Å
V = 1954.6 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.33 mm^{-1}
T = 296 (2) K
0.41 × 0.17 × 0.07 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: none
14721 measured reflections
4706 independent reflections
2807 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.099
S = 1.02
4706 reflections
254 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Absolute structure: Flack (1983), 1876 Friedel pairs
Flack parameter: −0.12 (7)

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O1^{i}	0.86	1.94	2.802 (3)	175
C7—H7A···N3^{ii}	0.93	2.54	3.446 (3)	164
C11—H11C···S1^{iii}	0.96	2.77	3.526 (3)	136
C20—H20A···O2^{iv}	0.93	2.48	3.380 (3)	162

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *APEX2*; software used to prepare material for publication: *APEX2* and *publCIF* (Westrip, 2008).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GW2052).

References

Bruker (2004). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Foroumadi, A., Daneshtalab, M. & Shafiee, A. (1999). *Arzneim. Forsch.* **49**, 1035–1038.
Fun, H.-K., Chantrapromma, S., Patil, P. S., Karthikeyan, M. S. & Dharmaprakash, S. M. (2008). *Acta Cryst.* E**64**, o956–o957.
Gowda, B. T., Tokarčík, M., Kožíšek, J., Sowmya, B. P. & Fuess, H. (2008). *Acta Cryst.* E**64**, o950.
Levy, M. & Palmer, A. H. (1942). *J. Biol. Chem.* **146**, 493–495.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Song, K. S., Ishikawa, Y., Kobayashi, S., Sankawa, U. & Ebizuka, Y. (1992). *Phytochemistry*, **31**, 823–826.
Thiruvalluvar, A., Subramanyam, M., Butcher, R. J., Karabasanagouda, T. & Adhikari, A. V. (2008). *Acta Cryst.* E**64**, o1263.
Tu, G. G., Li, S. H., Huang, H. M., Li, G., Xiong, F., Mai, X., Zhu, H. W., Kuang, B. H. & Xu, W. F. (2008). *Bioorg. Med. Chem.* **16**, 6663–6668.
Westrip, S. P. (2008). *publCIF*. In preparation.

‡ Additional correspondence author, e-mail: lishaohua0131@yahoo.com.cn.

supporting information

Acta Cryst. (2008). E**64**, o2006 [doi:10.1107/S1600536808030353]

(2*R*)-*N*-[5-(4-Chlorophenyl)-1,3,4-thiadiazol-2-yl]-2-(cinnamoylamino)-propanamide

Shao-Hua Li, Hui-Ming Huang, Bin-Hai Kuang, Guo-Gang Tu and Cheng-Mei Liu

S1. Comment

In our previous work, 1,3,4-thiadiazole scaffold compounds and their biological activity have been studied (Tu *et al.*, 2008). In view of the importance of these organic materials, the title compound (Fig. 1) was synthesized (Foroumadi *et al.*, 1999; Levy & Palmer 1942; Song *et al.*, 1992) and its crystal structure is reported here. The structure of title compound, $C_{20}H_{17}ClN_4O_2S$, has orthorhombic ($P2_12_12_1$) symmetry. The dihedral angles between the *p*-cholobenzene and thiadiazol rings is 3.4 (8) °, the corresponding values between the two benzene rings are measured to 65.9 (1)°. The conformations of the N—H and C=O bonds are anti with respect to each other. The enone groups are *trans* configurated. Bond lengths and angles are in normal ranges and comparable to those in related structures (Gowda *et al.*, 2008; Fun *et al.*, 2008; Thiruvalluvar *et al.*, 2008). In the crystal structure, molecules are linked through intermolecular hydrogen bonds forming a three-dimensional network (Table 1, Figure 2).

S2. Experimental

N,N-Dicyclohexylcarbodiimide (5.7 mmol) was added to a cooled solution of *N*-cinnamoyl-*D*-alanine (5.6 mmol) and *N*-hydroxysuccinimide (5.6 mmol) in freshly distillation dioxane (30 ml). The reaction mixture was stirred overnight at room temperature. The insoluble material was filtered off and washed with cold dioxane. 2-Amino-5-(4-choloxyphenyl)-1,3,4-thiadiazole (5.5 mmol) was added to the filtrate and the reaction mixture was stirred for 48 hr at room temperature. The solvent was removed under reduced pressure. The residual was dissolved in EtOAc and the insoluble material was filtered off. The filtrate was washed successively with saturated Na_2CO_3 solution(20 ml, *x* 3), water(20 ml, *x* 1), 0.1 *M* HCl(20 ml, *x* 3) and water(20 ml, *x* 1). The organic layer evaporated *in vacuo*, the residual was recrystallized from methanol. Colorless block-shaped single crystals of the title compound suitable for X-ray diffraction analysis precipitated after several days.

S3. Refinement

H atoms were positioned geometrically and refined using a riding model using *SHELXL97* default values (U_{iso}(H) = 1.2 U_{eq}(C) for CH and CH_2 groups and U_{iso}(H) = 1.5 U_{eq}(C) for CH_3). Refinement with all data (Friedel opposites not merged) led to an unsuitably large error of the Flack parameter. The final refinement was therefore performed with a data set with merged Friedel pairs, hence the calculated Flack parameter is meaningless. The absolute configuration is nevertheless undoubtly as described since enantiomerically pure starting compounds were used and the reaction conditions are not condidered to lead to racemization or inversion.

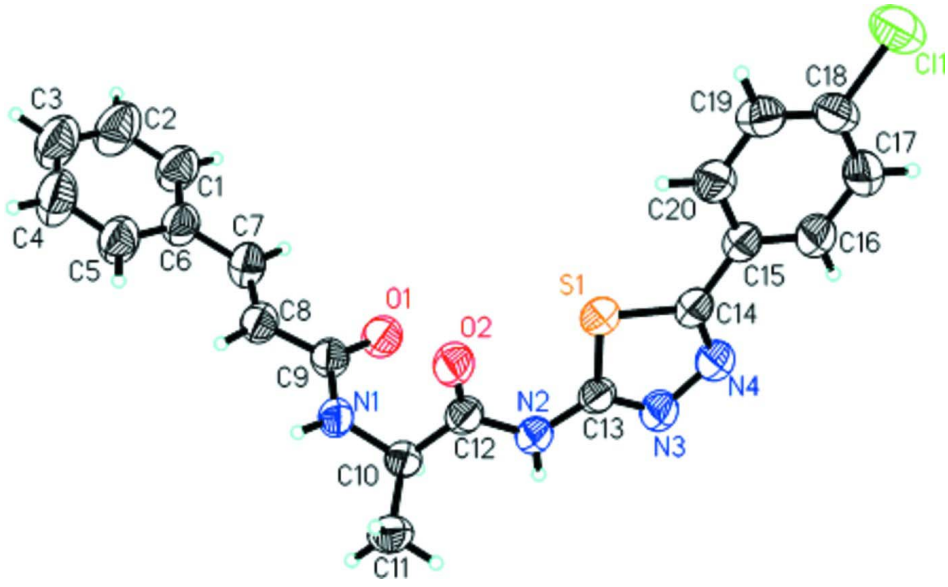


Figure 1

Molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

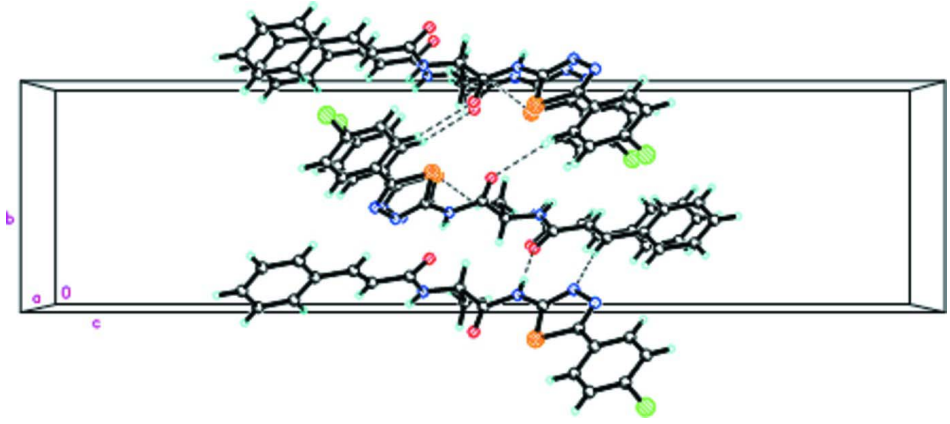


Figure 2

The crystal packing of title compound, viewed along the *a* axis with hydrogen bonds drawn as dashed lines.

(2*R*)-*N*-[5-(4-Chlorophenyl)-1,3,4-thiadiazol-2-yl]-2- (cinnamoylamino)propanamide

Crystal data

$C_{20}H_{17}ClN_4O_2S$
$M_r = 412.89$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 6.6324\ (15)$ Å
$b = 8.575\ (2)$ Å
$c = 34.367\ (8)$ Å
$V = 1954.6\ (8)$ Å^3
$Z = 4$
$F(000) = 856$
$D_x = 1.403$ Mg m^{-3}
Melting point: 480 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3308 reflections
$\theta = 2.4$–$21.0°$
$\mu = 0.33$ mm^{-1}
$T = 296$ K
Bolck, colourless
0.41 × 0.18 × 0.07 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
14721 measured reflections
4706 independent reflections
2807 reflections with $I > 2\sigma(I)$
$R_{int} = 0.046$
$\theta_{max} = 28.4°$, $\theta_{min} = 2.4°$
$h = -8 \rightarrow 8$
$k = -11 \rightarrow 11$
$l = -45 \rightarrow 44$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.099$
$S = 1.02$
4706 reflections
254 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
$w = 1/[\sigma^2(F_o^2) + (0.0226P)^2 + 0.0747P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.15$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ e Å^{-3}
Absolute structure: Flack (1983), 1876 Friedel pairs
Absolute structure parameter: −0.12 (7)

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}
C1	0.6789 (5)	0.2710 (4)	0.19355 (8)	0.0782 (9)
H1B	0.6067	0.2030	0.1777	0.094*
C2	0.6159 (6)	0.2979 (4)	0.23129 (10)	0.0996 (13)
H2B	0.5024	0.2468	0.2408	0.120*
C3	0.7184 (6)	0.3981 (5)	0.25465 (9)	0.0977 (12)
H3B	0.6745	0.4158	0.2800	0.117*
C4	0.8862 (6)	0.4732 (4)	0.24098 (8)	0.0937 (12)
H4B	0.9551	0.5434	0.2568	0.112*
C5	0.9526 (5)	0.4443 (4)	0.20360 (8)	0.0756 (9)
H5A	1.0692	0.4927	0.1947	0.091*
C6	0.8481 (5)	0.3443 (3)	0.17924 (7)	0.0613 (8)
C7	0.9087 (5)	0.3172 (3)	0.13882 (7)	0.0612 (8)
H7A	0.8246	0.2533	0.1242	0.073*
C8	1.0669 (4)	0.3722 (3)	0.12100 (7)	0.0584 (7)
H8A	1.1579	0.4314	0.1353	0.070*

C9	1.1094 (4)	0.3464 (3)	0.07984 (7)	0.0523 (7)
C10	1.3357 (4)	0.4044 (3)	0.02573 (6)	0.0483 (6)
H10A	1.3421	0.2934	0.0190	0.058*
C11	1.5445 (4)	0.4755 (3)	0.02035 (8)	0.0626 (8)
H11A	1.6384	0.4245	0.0374	0.094*
H11B	1.5397	0.5847	0.0264	0.094*
H11C	1.5870	0.4619	−0.0061	0.094*
C12	1.1836 (4)	0.4831 (3)	−0.00072 (7)	0.0494 (6)
C13	1.0385 (4)	0.4721 (3)	−0.06496 (7)	0.0471 (6)
C14	0.7573 (4)	0.5583 (3)	−0.10172 (6)	0.0494 (6)
C15	0.5693 (4)	0.6256 (3)	−0.11652 (7)	0.0490 (6)
C16	0.4931 (5)	0.5842 (3)	−0.15249 (7)	0.0639 (7)
H16A	0.5625	0.5115	−0.1675	0.077*
C17	0.3163 (5)	0.6479 (3)	−0.16687 (8)	0.0669 (8)
H17A	0.2679	0.6198	−0.1913	0.080*
C18	0.2142 (4)	0.7538 (3)	−0.14421 (8)	0.0589 (7)
C19	0.2848 (5)	0.7959 (3)	−0.10843 (8)	0.0637 (8)
H19A	0.2137	0.8676	−0.0935	0.076*
C20	0.4600 (4)	0.7328 (3)	−0.09455 (8)	0.0591 (7)
H20A	0.5068	0.7619	−0.0701	0.071*
Cl1	−0.00738 (13)	0.83679 (9)	−0.16181 (2)	0.0835 (3)
N1	1.2732 (3)	0.4188 (2)	0.06588 (5)	0.0537 (5)
H1A	1.3436	0.4758	0.0813	0.064*
N2	1.1824 (3)	0.4305 (2)	−0.03825 (5)	0.0525 (5)
H2A	1.2768	0.3681	−0.0455	0.063*
N3	1.0265 (4)	0.4021 (3)	−0.09856 (6)	0.0590 (6)
N4	0.8619 (4)	0.4535 (2)	−0.12001 (6)	0.0585 (6)
O1	1.0027 (3)	0.2679 (2)	0.05768 (5)	0.0672 (5)
O2	1.0712 (3)	0.5869 (2)	0.00979 (5)	0.0638 (5)
S1	0.85258 (10)	0.60793 (7)	−0.056449 (17)	0.05201 (18)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.081 (3)	0.090 (2)	0.0635 (18)	−0.017 (2)	0.0140 (18)	−0.0047 (16)
C2	0.112 (4)	0.116 (3)	0.070 (2)	−0.030 (3)	0.029 (2)	−0.004 (2)
C3	0.110 (3)	0.124 (3)	0.0594 (19)	−0.021 (3)	0.021 (2)	−0.006 (2)
C4	0.113 (3)	0.114 (3)	0.0541 (18)	−0.028 (3)	0.0073 (19)	−0.0090 (18)
C5	0.080 (2)	0.093 (2)	0.0539 (17)	−0.0173 (19)	0.0071 (16)	−0.0014 (15)
C6	0.068 (2)	0.0673 (18)	0.0484 (14)	−0.0030 (16)	0.0023 (14)	0.0034 (12)
C7	0.075 (2)	0.0623 (16)	0.0465 (15)	−0.0090 (16)	−0.0007 (15)	0.0002 (13)
C8	0.0591 (19)	0.0670 (17)	0.0490 (15)	−0.0077 (15)	0.0026 (13)	−0.0025 (13)
C9	0.0530 (19)	0.0535 (15)	0.0503 (14)	−0.0074 (13)	−0.0006 (13)	0.0012 (12)
C10	0.0448 (15)	0.0539 (14)	0.0464 (13)	−0.0036 (14)	0.0008 (12)	−0.0019 (11)
C11	0.0491 (19)	0.0728 (18)	0.0658 (17)	−0.0078 (15)	0.0092 (14)	−0.0079 (14)
C12	0.0496 (18)	0.0524 (15)	0.0460 (14)	−0.0044 (13)	0.0050 (12)	−0.0053 (11)
C13	0.0461 (16)	0.0516 (13)	0.0437 (13)	0.0004 (12)	0.0065 (12)	−0.0024 (11)
C14	0.0524 (18)	0.0529 (15)	0.0428 (13)	−0.0032 (13)	0.0074 (12)	−0.0003 (11)

C15	0.0502 (17)	0.0516 (14)	0.0453 (14)	−0.0025 (13)	0.0051 (12)	0.0000 (12)
C16	0.067 (2)	0.0747 (18)	0.0499 (15)	0.0125 (17)	0.0012 (15)	−0.0069 (13)
C17	0.065 (2)	0.081 (2)	0.0540 (15)	0.0083 (17)	−0.0075 (15)	−0.0055 (14)
C18	0.0460 (18)	0.0622 (17)	0.0686 (18)	0.0037 (14)	−0.0010 (14)	0.0109 (14)
C19	0.055 (2)	0.0669 (18)	0.0695 (18)	0.0050 (15)	0.0080 (15)	−0.0077 (14)
C20	0.056 (2)	0.0666 (17)	0.0545 (16)	0.0020 (16)	0.0009 (14)	−0.0103 (13)
Cl1	0.0582 (5)	0.0923 (6)	0.1001 (6)	0.0079 (4)	−0.0089 (5)	0.0129 (4)
N1	0.0521 (14)	0.0672 (13)	0.0417 (11)	−0.0115 (12)	−0.0006 (10)	−0.0046 (10)
N2	0.0508 (14)	0.0629 (13)	0.0439 (11)	0.0086 (11)	0.0030 (10)	−0.0048 (9)
N3	0.0611 (16)	0.0685 (13)	0.0472 (12)	0.0108 (13)	0.0006 (11)	−0.0074 (11)
N4	0.0591 (16)	0.0676 (13)	0.0488 (11)	0.0069 (13)	0.0014 (12)	−0.0090 (10)
O1	0.0605 (13)	0.0815 (12)	0.0595 (11)	−0.0230 (11)	0.0052 (11)	−0.0127 (10)
O2	0.0666 (13)	0.0715 (12)	0.0534 (10)	0.0174 (11)	−0.0024 (9)	−0.0166 (9)
S1	0.0507 (4)	0.0584 (4)	0.0469 (3)	0.0047 (3)	0.0040 (3)	−0.0059 (3)

Geometric parameters (Å, º)

C1—C6	1.377 (4)	C11—H11C	0.9600
C1—C2	1.382 (4)	C12—O2	1.216 (3)
C1—H1B	0.9300	C12—N2	1.367 (3)
C2—C3	1.359 (5)	C13—N3	1.304 (3)
C2—H2B	0.9300	C13—N2	1.372 (3)
C3—C4	1.369 (5)	C13—S1	1.721 (3)
C3—H3B	0.9300	C14—N4	1.298 (3)
C4—C5	1.380 (4)	C14—C15	1.465 (3)
C4—H4B	0.9300	C14—S1	1.732 (2)
C5—C6	1.384 (4)	C15—C16	1.382 (3)
C5—H5A	0.9300	C15—C20	1.393 (3)
C6—C7	1.465 (4)	C16—C17	1.385 (4)
C7—C8	1.303 (4)	C16—H16A	0.9300
C7—H7A	0.9300	C17—C18	1.375 (4)
C8—C9	1.459 (3)	C17—H17A	0.9300
C8—H8A	0.9300	C18—C19	1.364 (4)
C9—O1	1.239 (3)	C18—Cl1	1.741 (3)
C9—N1	1.340 (3)	C19—C20	1.368 (4)
C10—N1	1.446 (3)	C19—H19A	0.9300
C10—C12	1.517 (3)	C20—H20A	0.9300
C10—C11	1.524 (3)	N1—H1A	0.8600
C10—H10A	0.9800	N2—H2A	0.8600
C11—H11A	0.9600	N3—N4	1.389 (3)
C11—H11B	0.9600		
C6—C1—C2	120.4 (3)	H11B—C11—H11C	109.5
C6—C1—H1B	119.8	O2—C12—N2	121.2 (2)
C2—C1—H1B	119.8	O2—C12—C10	123.8 (2)
C3—C2—C1	120.6 (4)	N2—C12—C10	115.0 (2)
C3—C2—H2B	119.7	N3—C13—N2	121.0 (2)
C1—C2—H2B	119.7	N3—C13—S1	114.7 (2)

C2—C3—C4	120.1 (3)	N2—C13—S1	124.11 (17)
C2—C3—H3B	120.0	N4—C14—C15	124.0 (2)
C4—C3—H3B	120.0	N4—C14—S1	114.2 (2)
C3—C4—C5	119.6 (3)	C15—C14—S1	121.72 (18)
C3—C4—H4B	120.2	C16—C15—C20	117.6 (2)
C5—C4—H4B	120.2	C16—C15—C14	121.4 (2)
C4—C5—C6	121.0 (3)	C20—C15—C14	121.0 (2)
C4—C5—H5A	119.5	C15—C16—C17	121.8 (3)
C6—C5—H5A	119.5	C15—C16—H16A	119.1
C1—C6—C5	118.3 (3)	C17—C16—H16A	119.1
C1—C6—C7	119.3 (3)	C18—C17—C16	118.4 (3)
C5—C6—C7	122.3 (3)	C18—C17—H17A	120.8
C8—C7—C6	127.5 (3)	C16—C17—H17A	120.8
C8—C7—H7A	116.2	C19—C18—C17	121.1 (3)
C6—C7—H7A	116.2	C19—C18—Cl1	119.6 (2)
C7—C8—C9	123.8 (3)	C17—C18—Cl1	119.3 (2)
C7—C8—H8A	118.1	C18—C19—C20	120.1 (3)
C9—C8—H8A	118.1	C18—C19—H19A	120.0
O1—C9—N1	119.7 (2)	C20—C19—H19A	120.0
O1—C9—C8	124.6 (3)	C19—C20—C15	121.0 (3)
N1—C9—C8	115.7 (2)	C19—C20—H20A	119.5
N1—C10—C12	110.1 (2)	C15—C20—H20A	119.5
N1—C10—C11	110.0 (2)	C9—N1—C10	122.3 (2)
C12—C10—C11	110.7 (2)	C9—N1—H1A	118.8
N1—C10—H10A	108.7	C10—N1—H1A	118.8
C12—C10—H10A	108.7	C12—N2—C13	123.3 (2)
C11—C10—H10A	108.7	C12—N2—H2A	118.3
C10—C11—H11A	109.5	C13—N2—H2A	118.3
C10—C11—H11B	109.5	C13—N3—N4	111.8 (2)
H11A—C11—H11B	109.5	C14—N4—N3	112.5 (2)
C10—C11—H11C	109.5	C13—S1—C14	86.70 (12)
H11A—C11—H11C	109.5		

C6—C1—C2—C3	0.7 (6)	C16—C17—C18—C19	0.2 (4)
C1—C2—C3—C4	−0.3 (6)	C16—C17—C18—Cl1	179.5 (2)
C2—C3—C4—C5	−1.2 (6)	C17—C18—C19—C20	0.1 (4)
C3—C4—C5—C6	2.2 (5)	Cl1—C18—C19—C20	−179.2 (2)
C2—C1—C6—C5	0.2 (5)	C18—C19—C20—C15	0.2 (4)
C2—C1—C6—C7	−178.4 (3)	C16—C15—C20—C19	−0.8 (4)
C4—C5—C6—C1	−1.7 (5)	C14—C15—C20—C19	179.8 (2)
C4—C5—C6—C7	176.8 (3)	O1—C9—N1—C10	−2.3 (4)
C1—C6—C7—C8	−177.5 (3)	C8—C9—N1—C10	179.8 (2)
C5—C6—C7—C8	4.0 (5)	C12—C10—N1—C9	67.6 (3)
C6—C7—C8—C9	−176.3 (2)	C11—C10—N1—C9	−170.1 (2)
C7—C8—C9—O1	−1.3 (4)	O2—C12—N2—C13	−9.9 (4)
C7—C8—C9—N1	176.5 (3)	C10—C12—N2—C13	171.0 (2)
N1—C10—C12—O2	24.2 (3)	N3—C13—N2—C12	−170.0 (2)
C11—C10—C12—O2	−97.7 (3)	S1—C13—N2—C12	5.7 (3)

N1—C10—C12—N2	−156.8 (2)	N2—C13—N3—N4	175.5 (2)
C11—C10—C12—N2	81.4 (3)	S1—C13—N3—N4	−0.5 (3)
N4—C14—C15—C16	−2.3 (4)	C15—C14—N4—N3	−176.1 (2)
S1—C14—C15—C16	−179.3 (2)	S1—C14—N4—N3	1.1 (3)
N4—C14—C15—C20	177.1 (2)	C13—N3—N4—C14	−0.4 (3)
S1—C14—C15—C20	0.1 (3)	N3—C13—S1—C14	0.9 (2)
C20—C15—C16—C17	1.1 (4)	N2—C13—S1—C14	−175.0 (2)
C14—C15—C16—C17	−179.5 (2)	N4—C14—S1—C13	−1.2 (2)
C15—C16—C17—C18	−0.8 (4)	C15—C14—S1—C13	176.1 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O1^{i}	0.86	1.94	2.802 (3)	175
C7—H7*A*···O1	0.93	2.58	2.888 (3)	100
C7—H7*A*···N3^{ii}	0.93	2.54	3.446 (3)	164
C11—H11*C*···S1^{iii}	0.96	2.77	3.526 (3)	136
C20—H20*A*···S1	0.93	2.69	3.105 (3)	108
C20—H20*A*···O2^{iv}	0.93	2.48	3.380 (3)	162

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