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(*E*)-2-(3-Cinnamoylthioureido)acetic acid dimethyl sulfoxide disolvate

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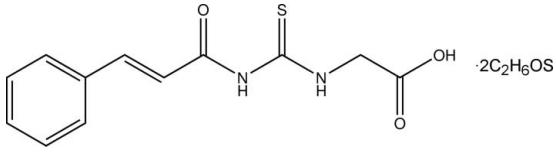
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.010 Å; R factor = 0.085; wR factor = 0.251; data-to-parameter ratio = 15.7.

In the title compound, $C_{12}H_{12}N_2O_3S\cdot 2C_2H_6OS$, the acetic acid and cinnamoyl groups adopt Z and E configurations, respectively, with respect to the thio group about the C—N bonds. The components of the asymmetric unit are connected by N—H···O and O—H···O hydrogen bonds and in the crystal weak intermolecular C—H···O and C—H···S hydrogen bonds further connect the components into chains along the b axis. In the main molecule, an intramolecular N—H···O hydrogen bond is also present.

Related literature

For related structures, see: Hassan *et al.* (2009, 2010*a*,*b*,*c*, 2011); Nasir *et al.* (2011). For the synthesis, see: Hassan *et al.* (2008). For standard bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{12}H_{12}N_2O_3S\cdot 2C_2H_6OS$
M_r = 420.55
Triclinic, $P\overline{1}$
a = 7.327 (3) Å
b = 12.064 (5) Å
c = 13.691 (6) Å
α = 65.794 (8)°
β = 75.603 (9)°
γ = 85.484 (9)°
V = 1068.6 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.37 mm^{-1}
T = 298 K
0.42 × 0.21 × 0.18 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.859, T_{max} = 0.936
10964 measured reflections
3774 independent reflections
2650 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.085
$wR(F^2)$ = 0.251
S = 1.06
3774 reflections
240 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.72 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*A*···O5	0.86	2.02	2.867 (5)	167
N2—H2*A*···O1	0.86	1.94	2.625 (4)	136
O3—H3*A*···O4	0.82	1.76	2.562 (5)	166
C14—H14*C*···O2	0.96	2.54	3.423 (8)	153
C14—H14*A*···O5^{i}	0.96	2.43	3.319 (7)	154
C15—H15*B*···O4^{ii}	0.96	2.58	3.468 (7)	153
C16—H16*B*···S1^{iii}	0.96	2.85	3.702 (7)	148

Symmetry codes: (i) $x, y+1, z$; (ii) $-x+1, -y+2, -z+1$; (iii) $-x+1, -y+1, -z+1$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996) and *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5324).

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supporting information

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(*E*)-2-(3-Cinnamoylthioureido)acetic acid dimethyl sulfoxide disolvate

Ibrahim N. Hassan, Wan Ramli Wan Daud, Bohari M. Yamin and Mohammad B. Kassim

S1. Comment

The title compound (I) is the thiourea carboxylic acid version of our previously reported ester molecules *(E)*-methyl-2-(3-cinnamoylthioureido)acetate (II) (Hassan *et al.*, 2010*a*)and *(E)*-ethyl-2-(3- cinnmoylthioureido)acetate (III) (Hassan *et al.*, 2010*b*) and analogous to methyl-2-(3-benzoylthioureido)acetate (IV) (Hassan *et al.*, 2009). The molecule maintains the same *E-Z* configuration with respect to the positions of the acetic acid and cinnamoyl groups, relative to the S atom across the C—N bonds, respectively (Fig. 1). In general, the bond lengths (Allen *et al.*, 1987) and angles in (I) are in normal ranges and comparable to those in (II), (III) and (IV). The the C═S bond length [1.665 (4) Å] is the same within experimental error to that in (II) [1.666 (3) Å] and that of (III) [1.656 (5) Å]. The C7═C8 bond length [1.331 (6) Å] is slightly longer than that reported by Hassan *et al.* (2010*c*) [1.320 (3) Å]. The carbonyl C═O bond length [1.215 (5) Å] is the same within experimental error to that reported by Nasir *et al.* (2011) [1.213 (3) Å]. The S1/O1/O2/N1/N2/C1—C12 fragment is essentially planar with a maximum deviation of 0.043 (5) Å, for atom C7. In the crystal, the components of the asymmtric unit are connected by N—H···O and O—H···O hydrogen bonds and weak intermolecular C—H···O and C—H···S hydrogen bonds connect the components into one-dimensional chains along the *b* axis (Fig. 2). In the main molecule an intramolecular N—H···O hydrogen bond is also present.

S2. Experimental

The title compound was synthesized according to a previously reported method (Hassan *et al.*, 2008). A yellowish crystal, suitable for X-ray crystallography, was obtained by a slow evaporation from CH_2Cl_2 solution at room temperature (yield 79%).

S3. Refinement

All H atoms were positioned geometrically and allowed to ride on their parent atoms with C—H = 0.93-0.97Å, N—H = 0.86Å and O—H = 0.82Å and with $U_{iso}(H) = 1.2U_{eq}(C,N)$ or $1.5U_{eq}(C_{methyl},O)$.

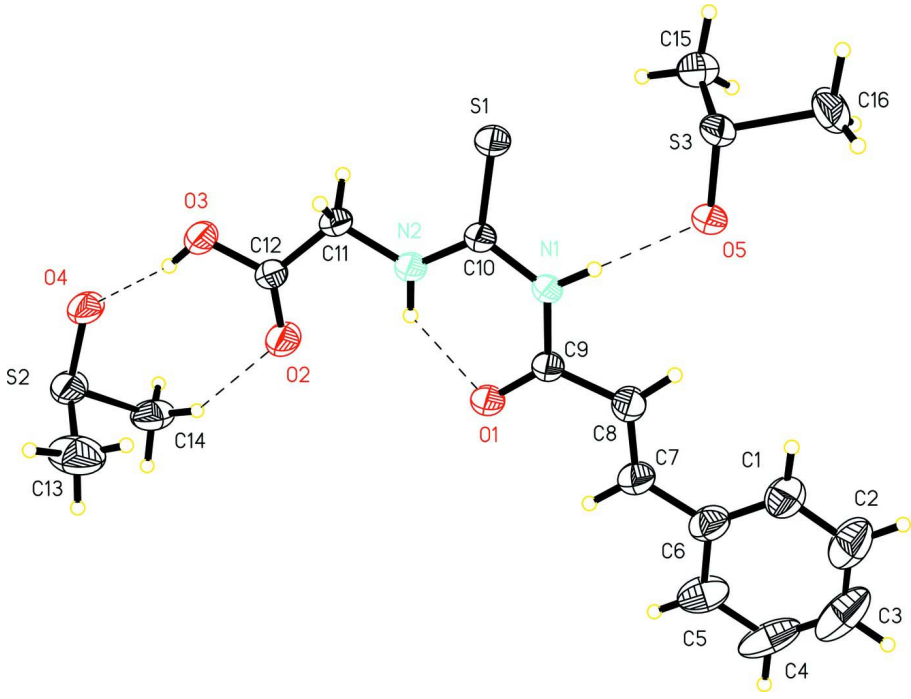

Figure 1

The molecular structure of (I), with displacement ellipsoids are drawn at the 50% probability level. Hydrogen bonds are shown as dashed lines.

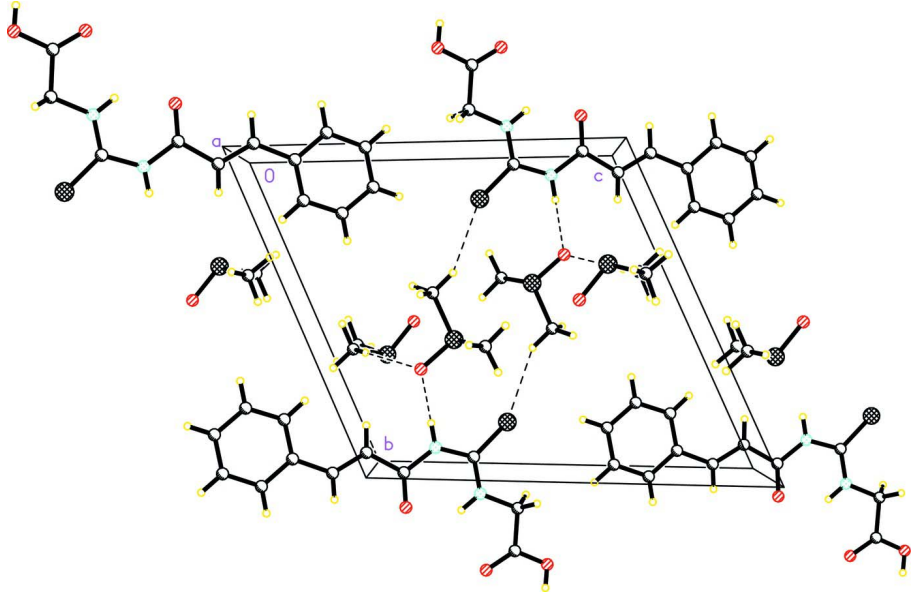

Figure 2

A packing diagram of (I) viewed along the *c* axis. Hydrogen bonds are shown by dashed lines.

(*E*)-2-(3-Cinnamoylthioureido)acetic acid dimethyl sulfoxide disolvate

Crystal data

$C_{12}H_{12}N_2O_3S·2C_2H_6OS$
$M_r = 420.55$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.327$ (3) Å
$b = 12.064$ (5) Å
$c = 13.691$ (6) Å
$\alpha = 65.794$ (8)°
$\beta = 75.603$ (9)°
$\gamma = 85.484$ (9)°
$V = 1068.6$ (8) Å^3
$Z = 2$
$F(000) = 444$
$D_x = 1.307$ Mg m^{-3}
Melting point: 407 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$\theta = 1.7$–25.0°
$\mu = 0.37$ mm^{-1}
$T = 298$ K
Block, colourless
0.42 × 0.21 × 0.18 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.859$, $T_{max} = 0.936$
10964 measured reflections
3774 independent reflections
2650 reflections with $I > 2\sigma(I)$
$R_{int} = 0.046$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.7°$
$h = -8 \rightarrow 8$
$k = -14 \rightarrow 14$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.085$
$wR(F^2) = 0.251$
$S = 1.06$
3774 reflections
240 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
$w = 1/[\sigma^2(F_o^2) + (0.1544P)^2 + 0.4047P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.72$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.4518 (2)	0.84669 (10)	0.40846 (9)	0.0689 (5)
S2	0.3003 (3)	1.64039 (11)	0.16460 (11)	0.0800 (6)
S3	0.66629 (18)	0.58770 (10)	0.36710 (9)	0.0580 (4)

O1	0.6554 (5)	1.1084 (3)	0.0515 (2)	0.0642 (10)
O2	0.4605 (6)	1.3125 (3)	0.1829 (3)	0.0754 (11)
O3	0.2971 (6)	1.3022 (3)	0.3467 (3)	0.0697 (11)
H3A	0.3008	1.3765	0.3147	0.105*
O4	0.2660 (7)	1.5335 (3)	0.2747 (3)	0.0836 (13)
O5	0.7343 (5)	0.6780 (3)	0.2502 (2)	0.0626 (9)
N1	0.6120 (5)	0.9232 (3)	0.1959 (3)	0.0457 (9)
H1A	0.6309	0.8470	0.2128	0.055*
N2	0.4931 (5)	1.0710 (3)	0.2566 (3)	0.0495 (9)
H2A	0.5327	1.1210	0.1891	0.059*
C1	0.9539 (8)	0.8304 (6)	−0.1493 (5)	0.0762 (16)
H1	0.9122	0.7733	−0.0774	0.091*
C2	1.0432 (9)	0.7939 (8)	−0.2298 (6)	0.097 (2)
H2	1.0635	0.7115	−0.2118	0.116*
C3	1.1037 (10)	0.8736 (11)	−0.3359 (8)	0.116 (3)
H3	1.1623	0.8466	−0.3903	0.139*
C4	1.0773 (10)	0.9927 (10)	−0.3607 (5)	0.105 (3)
H4	1.1197	1.0486	−0.4331	0.126*
C5	0.9890 (8)	1.0335 (7)	−0.2812 (4)	0.0843 (18)
H5	0.9724	1.1163	−0.2998	0.101*
C6	0.9249 (7)	0.9513 (5)	−0.1739 (4)	0.0648 (13)
C7	0.8281 (7)	0.9974 (5)	−0.0920 (4)	0.0618 (13)
H7A	0.8061	1.0803	−0.1186	0.074*
C8	0.7671 (7)	0.9352 (4)	0.0163 (4)	0.0608 (13)
H8A	0.7811	0.8514	0.0475	0.073*
C9	0.6774 (6)	0.9993 (4)	0.0869 (3)	0.0492 (11)
C10	0.5195 (6)	0.9548 (4)	0.2819 (3)	0.0444 (10)
C11	0.4015 (7)	1.1193 (4)	0.3357 (3)	0.0491 (11)
H11A	0.4714	1.0991	0.3921	0.059*
H11B	0.2754	1.0838	0.3711	0.059*
C12	0.3910 (6)	1.2548 (4)	0.2786 (3)	0.0492 (11)
C13	0.1632 (10)	1.6099 (7)	0.0894 (5)	0.106 (2)
H13A	0.1832	1.5281	0.0948	0.159*
H13B	0.1992	1.6657	0.0134	0.159*
H13C	0.0324	1.6191	0.1188	0.159*
C14	0.5210 (8)	1.6206 (5)	0.0879 (4)	0.0731 (15)
H14A	0.6180	1.6301	0.1201	0.110*
H14B	0.5404	1.6803	0.0134	0.110*
H14C	0.5254	1.5407	0.0884	0.110*
C15	0.8192 (9)	0.6064 (6)	0.4402 (4)	0.0790 (16)
H15A	0.9473	0.6011	0.4033	0.118*
H15B	0.7928	0.5438	0.5136	0.118*
H15C	0.8011	0.6846	0.4436	0.118*
C16	0.7496 (11)	0.4446 (5)	0.3663 (5)	0.093 (2)
H16A	0.6882	0.4229	0.3220	0.139*
H16B	0.7219	0.3834	0.4403	0.139*
H16C	0.8833	0.4507	0.3360	0.139*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.1061 (11)	0.0398 (7)	0.0338 (6)	0.0062 (6)	0.0081 (6)	−0.0032 (5)
S2	0.1332 (14)	0.0414 (7)	0.0428 (7)	0.0122 (7)	−0.0026 (7)	−0.0070 (6)
S3	0.0743 (8)	0.0416 (6)	0.0401 (6)	0.0072 (5)	−0.0023 (5)	−0.0063 (5)
O1	0.101 (3)	0.0401 (17)	0.0329 (16)	0.0086 (16)	−0.0024 (16)	−0.0054 (13)
O2	0.125 (3)	0.0399 (17)	0.0402 (19)	0.0064 (18)	0.0049 (19)	−0.0102 (15)
O3	0.115 (3)	0.0444 (18)	0.0399 (17)	0.0144 (19)	−0.0037 (18)	−0.0176 (15)
O4	0.148 (4)	0.0432 (19)	0.0376 (18)	0.017 (2)	0.000 (2)	−0.0100 (15)
O5	0.100 (3)	0.0400 (16)	0.0360 (17)	0.0079 (16)	−0.0103 (16)	−0.0081 (14)
N1	0.069 (2)	0.0281 (16)	0.0323 (17)	0.0028 (15)	−0.0075 (16)	−0.0075 (14)
N2	0.071 (2)	0.0331 (18)	0.0317 (18)	0.0024 (16)	−0.0019 (16)	−0.0070 (14)
C1	0.076 (4)	0.087 (4)	0.063 (3)	0.011 (3)	−0.005 (3)	−0.036 (3)
C2	0.079 (4)	0.133 (6)	0.102 (6)	0.017 (4)	−0.012 (4)	−0.079 (5)
C3	0.078 (5)	0.205 (10)	0.105 (6)	−0.006 (6)	0.001 (4)	−0.114 (7)
C4	0.087 (5)	0.180 (9)	0.043 (3)	−0.043 (5)	0.013 (3)	−0.049 (5)
C5	0.083 (4)	0.105 (5)	0.041 (3)	−0.022 (3)	0.010 (3)	−0.016 (3)
C6	0.061 (3)	0.083 (4)	0.048 (3)	0.002 (3)	−0.005 (2)	−0.028 (3)
C7	0.080 (3)	0.057 (3)	0.040 (2)	0.002 (2)	−0.005 (2)	−0.016 (2)
C8	0.080 (3)	0.044 (3)	0.046 (3)	0.002 (2)	−0.002 (2)	−0.014 (2)
C9	0.066 (3)	0.038 (2)	0.034 (2)	0.0030 (19)	−0.004 (2)	−0.0099 (18)
C10	0.058 (3)	0.036 (2)	0.035 (2)	0.0030 (18)	−0.0094 (19)	−0.0114 (17)
C11	0.065 (3)	0.044 (2)	0.030 (2)	0.004 (2)	−0.0035 (19)	−0.0121 (18)
C12	0.068 (3)	0.044 (2)	0.035 (2)	0.006 (2)	−0.011 (2)	−0.0163 (19)
C13	0.091 (5)	0.121 (6)	0.063 (4)	−0.011 (4)	−0.010 (3)	0.004 (4)
C14	0.095 (4)	0.069 (3)	0.042 (3)	−0.011 (3)	−0.011 (3)	−0.010 (2)
C15	0.097 (4)	0.079 (4)	0.049 (3)	0.020 (3)	−0.015 (3)	−0.019 (3)
C16	0.130 (5)	0.037 (3)	0.076 (4)	0.007 (3)	0.008 (4)	−0.007 (3)

Geometric parameters (Å, º)

S1—C10	1.664 (4)	C4—C5	1.372 (9)
S2—O4	1.506 (3)	C4—H4	0.9300
S2—C14	1.754 (6)	C5—C6	1.378 (7)
S2—C13	1.757 (7)	C5—H5	0.9300
S3—O5	1.501 (3)	C6—C7	1.457 (7)
S3—C15	1.758 (6)	C7—C8	1.331 (6)
S3—C16	1.789 (6)	C7—H7A	0.9300
O1—C9	1.215 (5)	C8—C9	1.477 (6)
O2—C12	1.199 (5)	C8—H8A	0.9300
O3—C12	1.313 (5)	C11—C12	1.500 (6)
O3—H3A	0.8200	C11—H11A	0.9700
N1—C9	1.375 (5)	C11—H11B	0.9700
N1—C10	1.386 (5)	C13—H13A	0.9600
N1—H1A	0.8600	C13—H13B	0.9600
N2—C10	1.310 (5)	C13—H13C	0.9600
N2—C11	1.434 (5)	C14—H14A	0.9600

N2—H2A	0.8600	C14—H14B	0.9600
C1—C2	1.353 (8)	C14—H14C	0.9600
C1—C6	1.368 (8)	C15—H15A	0.9600
C1—H1	0.9300	C15—H15B	0.9600
C2—C3	1.353 (12)	C15—H15C	0.9600
C2—H2	0.9300	C16—H16A	0.9600
C3—C4	1.344 (13)	C16—H16B	0.9600
C3—H3	0.9300	C16—H16C	0.9600

O4—S2—C14	106.8 (3)	O1—C9—C8	123.3 (4)
O4—S2—C13	105.6 (3)	N1—C9—C8	113.7 (4)
C14—S2—C13	97.0 (3)	N2—C10—N1	116.2 (3)
O5—S3—C15	105.7 (3)	N2—C10—S1	124.2 (3)
O5—S3—C16	104.9 (2)	N1—C10—S1	119.6 (3)
C15—S3—C16	97.7 (3)	N2—C11—C12	109.5 (3)
C12—O3—H3A	109.5	N2—C11—H11A	109.8
C9—N1—C10	127.7 (3)	C12—C11—H11A	109.8
C9—N1—H1A	116.1	N2—C11—H11B	109.8
C10—N1—H1A	116.1	C12—C11—H11B	109.8
C10—N2—C11	123.4 (3)	H11A—C11—H11B	108.2
C10—N2—H2A	118.3	O2—C12—O3	124.4 (4)
C11—N2—H2A	118.3	O2—C12—C11	124.1 (4)
C2—C1—C6	119.9 (6)	O3—C12—C11	111.5 (4)
C2—C1—H1	120.0	S2—C13—H13A	109.5
C6—C1—H1	120.0	S2—C13—H13B	109.5
C1—C2—C3	122.0 (8)	H13A—C13—H13B	109.5
C1—C2—H2	119.0	S2—C13—H13C	109.5
C3—C2—H2	119.0	H13A—C13—H13C	109.5
C4—C3—C2	118.5 (6)	H13B—C13—H13C	109.5
C4—C3—H3	120.8	S2—C14—H14A	109.5
C2—C3—H3	120.8	S2—C14—H14B	109.5
C3—C4—C5	121.3 (7)	H14A—C14—H14B	109.5
C3—C4—H4	119.4	S2—C14—H14C	109.5
C5—C4—H4	119.4	H14A—C14—H14C	109.5
C4—C5—C6	119.7 (7)	H14B—C14—H14C	109.5
C4—C5—H5	120.1	S3—C15—H15A	109.5
C6—C5—H5	120.1	S3—C15—H15B	109.5
C1—C6—C5	118.5 (5)	H15A—C15—H15B	109.5
C1—C6—C7	123.1 (5)	S3—C15—H15C	109.5
C5—C6—C7	118.4 (5)	H15A—C15—H15C	109.5
C8—C7—C6	127.9 (5)	H15B—C15—H15C	109.5
C8—C7—H7A	116.0	S3—C16—H16A	109.5
C6—C7—H7A	116.0	S3—C16—H16B	109.5
C7—C8—C9	119.9 (4)	H16A—C16—H16B	109.5
C7—C8—H8A	120.0	S3—C16—H16C	109.5
C9—C8—H8A	120.0	H16A—C16—H16C	109.5
O1—C9—N1	122.9 (4)	H16B—C16—H16C	109.5

C6—C1—C2—C3	−0.9 (10)	C10—N1—C9—O1	−2.1 (8)
C1—C2—C3—C4	1.5 (12)	C10—N1—C9—C8	−179.0 (4)
C2—C3—C4—C5	−0.8 (12)	C7—C8—C9—O1	−0.2 (8)
C3—C4—C5—C6	−0.3 (11)	C7—C8—C9—N1	176.6 (4)
C2—C1—C6—C5	−0.2 (9)	C11—N2—C10—N1	−179.4 (4)
C2—C1—C6—C7	179.3 (6)	C11—N2—C10—S1	−0.1 (7)
C4—C5—C6—C1	0.8 (9)	C9—N1—C10—N2	−0.9 (7)
C4—C5—C6—C7	−178.7 (6)	C9—N1—C10—S1	179.8 (4)
C1—C6—C7—C8	5.5 (9)	C10—N2—C11—C12	−178.7 (4)
C5—C6—C7—C8	−175.0 (6)	N2—C11—C12—O2	−4.4 (7)
C6—C7—C8—C9	177.8 (5)	N2—C11—C12—O3	175.8 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O5	0.86	2.02	2.867 (5)	167
N2—H2*A*···O1	0.86	1.94	2.625 (4)	136
O3—H3*A*···O4	0.82	1.76	2.562 (5)	166
C14—H14*C*···O2	0.96	2.54	3.423 (8)	153
C14—H14*A*···O5^{i}	0.96	2.43	3.319 (7)	154
C15—H15*B*···O4^{ii}	0.96	2.58	3.468 (7)	153
C16—H16*B*···S1^{iii}	0.96	2.85	3.702 (7)	148

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