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Crystal structure of ethyl 3-anilino-2-{[bis(methylsulfanyl)methylidene]-amino}-3-oxopropanoate

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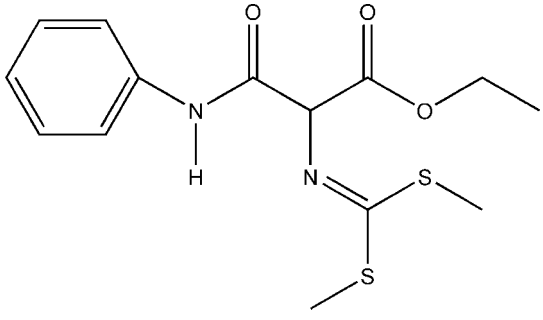
The molecular conformation of the title compound, $C_{14}H_{18}N_2O_3S_2$, is stabilized by intramolecular N—H···N and C—H···O hydrogen bonds. The crystal packing is characterized by a series of C—H···O hydrogen bonds, resulting in a three-dimensional network.

Keywords: crystal structure; thiazolo[5,4-*b*]quinoline derivative; hydrogen bonding.

CCDC reference: 1014381

1. Related literature

For the synthesis and cytotoxic activity of thiazolo[5,4-*b*]quinoline derivatives, see: Rodríguez-Loaiza *et al.* (2004); Loza-Mejía *et al.* (2008, 2009); Adams *et al.* (2002).



2. Experimental

2.1. Crystal data

$C_{14}H_{18}N_2O_3S_2$
M_r = 326.42
Triclinic, $P\overline{1}$
a = 8.5298 (11) Å
b = 9.1422 (16) Å
c = 11.0268 (13) Å
α = 101.377 (12)°
β = 102.102 (10)°
γ = 104.457 (13)°
V = 785.3 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.35 mm^{-1}
T = 145 K
0.6 × 0.5 × 0.35 mm

2.2. Data collection

Agilent Xcalibur Atlas Gemini diffractometer
Absorption correction: analytical (*CrysAlis RED*; Agilent, 2012)
T_{min} = 0.87, T_{max} = 0.922
5879 measured reflections
3625 independent reflections
3022 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.101
S = 1.05
3625 reflections
197 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*F*···N2	0.889 (15)	2.019 (18)	2.586 (2)	120.5 (15)
C2—H2···O1	0.95	2.33	2.932 (2)	121
C6—H6···O2^{i}	0.95	2.4	3.295 (2)	156
C10—H10*B*···O1^{ii}	0.99	2.53	3.340 (2)	138
C10—H10*B*···O3^{ii}	0.99	2.65	3.377 (2)	131
C11—H11*A*···O2^{iii}	0.98	2.64	3.465 (2)	141
C13—H13*B*···O1^{iv}	0.98	2.63	3.579 (2)	162

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

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Agilent, 2012); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

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Supporting information for this paper is available from the IUCr electronic archives (Reference: BT6988).

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Crystal structure of ethyl 3-anilino-2-{[bis(methylsulfanyl)methylidene]amino}-3-oxopropanoate

A. Kémish López-Rodríguez, Alfonso Lira-Rocha and Marcos Flores-Alamo

S1. Comment

Quinoline fused five-membered heterocyclic compounds have been the subject of sustained interest because many of them have cytotoxic properties. Thus, they are potential antitumor agents (Adams *et al.*, 2002). We have reported the synthesis and cytotoxic activity of several thiazolo[5,4-*b*]quinoline (TQ) derivatives (Rodríguez-Loaiza *et al.*, 2004; Loza-Mejía *et al.*, 2008; Loza-Mejía *et al.*, 2009.). During a study on the synthesis of new oxazolo[5,4-*b*]quinoline derivatives, which can be considered as analogues of TQ, the preparation of a key intermediate was tried by using a procedure previously reported by our group.

In the title compound, the asymmetric unit consist of one molecule of the ethyl-2-{[bis(methylsulfanyl)methylidene]amino}-3-oxo-3-(phenylamino)-propanoate (Fig. 1). The planes formed by phenyl ring C1/C6 (equation plane: 6.499 (4) *x* + 3.679 (6) *y* - 5.701 (6) *z* = 0.613 (6)) and the N1—C7/O1—C8 group (equation plane: 6.941 (4) *x* + 3.217 (7) *y* - 4.499 (8) *z* = 1.040 (4)) are almost coplanar with a dihedral angle between them of 7.64 (11)°; of the same way the dihedral angle of 8.34 (9)° between planes formed by N1—C7/O1—C8 and S1—C12/N2—S2 (equation plane: 7.465 (2) *x* + 2.049 (5) *y* - 4.965 (2) *z* = 0.633 (9)) evidence the coplanarity. On the other hand, the plane formed by C8—C9/O2—O3 (equation plane: - 3.115 (6) *x* + 8.551 (3) *y* + 1.760 (9) *z* = 3.314 (1)) shows a behavior near to orthogonality with the other planes.

In the crystal structure there are intermolecular C—H···O contacts (Table 1) connecting the molecules to a three-dimensional network.

S2. Experimental

Ethyl {[bis(methylsulfanyl)methylidene]amino}acetate was reacted with phenyl isocyanate at low temperature (-75°) under basic conditions, in order to obtain the oxazole derivative which is a intermediate suitable for the formation of the oxazolo[5,4-*b*]quinoline system. Surprisingly, this reaction gave in a high yield a different crystal intermediate, whose structure was characterized by IR, NMR and X-ray studies. Yield: 66.7%. Colorless crystals; mp: 103°C; IR (*v*max, cm^{-1}): 3283 (–NH amidic); 2982, 2930, 2891 (–CH aliph.); 1733 (C=O ester); 1687 (C=O amidic); 1H NMR (400 MHz, DMSO-*d* $_6$): d 1.17 (t, *J* = 7.1 Hz, 3H) $–CH_3$; 2.46 (s, 3H) $–SCH_3$; 2.59 (s, 3H) $–SCH_3$; 4.14 (q, *J* = 7.1, 2H) $–CH_2$; 5.00 (s, 1H) –CH; 7.07 (t, *J* = 7.8 Hz, 1H) –H4; 7.31 (d, *J* = 7.8 Hz, 2H) –H3, –H5; 7.61 (d, J = 8.4 Hz, 2H) –H2, –H6; 9.97 (s, 1H) –NH–; ^{13}C NMR (101 MHz, DMSO– *d* $_6$): d 14.42, 14.98, 15.26, 61.69, 69.68, 120.03, 124.33, 129.20, 138.74, 165.34, 167.06.

S3. Refinement

The H atom of the amine group (N1/H1F) was located in a difference map and refined isotropically with U_{iso}(H) = 1.2U_{eq}(N). The N-H distance was restrained to 0.92 (2)Å. H atoms attached to C atoms were placed in geometrically

idealized positions and refined as riding on their parent atoms, with C—H = 0.95–0.99 Å and with U_{iso}(H) = 1.2U_{eq}(C), for aromatic and methylene groups and U_{iso}(H) = 1.5U_eq(C) for methyl groups.

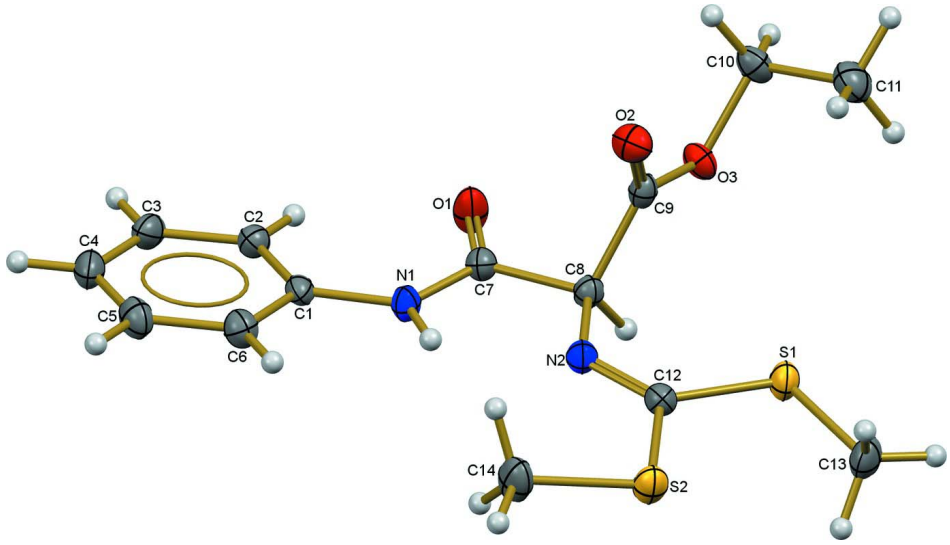

Figure 1

The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as circles of arbitrary size.

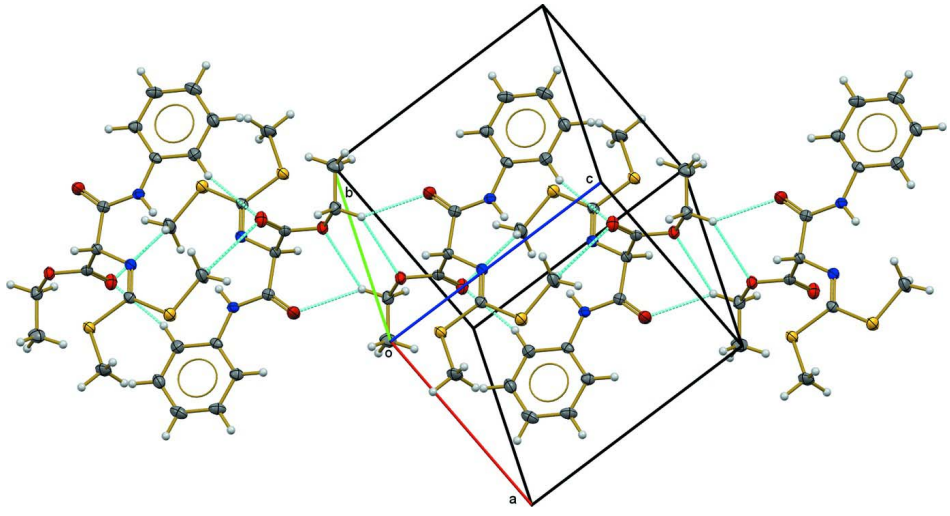

Figure 2

Crystal packing with intermolecular interactions of type C—H···O forming a three-dimensional network.

Ethyl 3-anilino-2-{[bis(methylsulfanyl)methylidene]amino}-3-oxopropanoate

Crystal data

$C_{14}H_{18}N_2O_3S_2$
M_r = 326.42
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 8.5298 (11) Å
b = 9.1422 (16) Å
c = 11.0268 (13) Å
α = 101.377 (12)°
β = 102.102 (10)°
γ = 104.457 (13)°
V = 785.3 (2) Å^3
Z = 2
F(000) = 344
D_x = 1.38 Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2290 reflections
θ = 3.6–29.4°
μ = 0.35 mm^{-1}

T = 145 K
Block, colourless
0.6 × 0.5 × 0.35 mm

Data collection

Agilent Xcalibur Atlas Gemini diffractometer
Graphite monochromator
Detector resolution: 10.4685 pixels mm^{-1}
ω scans
Absorption correction: analytical (*CrysAlis RED*; Agilent, 2012)
T_{min} = 0.87, T_{max} = 0.922

5879 measured reflections
3625 independent reflections
3022 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 29.4°, θ_{min} = 3.6°
h = −11→11
k = −9→11
l = −15→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.101
S = 1.05
3625 reflections
197 parameters
1 restraint

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0448P)^2 + 0.1551P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.033 (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.

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

	x	y	z	U_{iso}*/U_{eq}
C1	0.22485 (19)	0.68715 (19)	0.59186 (14)	0.0184 (3)
C2	0.1478 (2)	0.8032 (2)	0.57936 (16)	0.0216 (4)
H2	0.0786	0.7997	0.4985	0.026*
C3	0.1738 (2)	0.9243 (2)	0.68710 (16)	0.0260 (4)
H3	0.1217	1.0038	0.6792	0.031*
C4	0.2741 (2)	0.9311 (2)	0.80562 (17)	0.0289 (4)
H4	0.2909	1.0146	0.8784	0.035*
C5	0.3498 (2)	0.8150 (2)	0.81709 (16)	0.0276 (4)
H5	0.4188	0.819	0.8981	0.033*
C6	0.3254 (2)	0.6930 (2)	0.71085 (16)	0.0241 (4)
H6	0.3773	0.6135	0.7193	0.029*
C7	0.13582 (19)	0.5349 (2)	0.36177 (15)	0.0194 (3)
C8	0.1513 (2)	0.38584 (19)	0.27795 (14)	0.0187 (3)
H8	0.0362	0.3141	0.2294	0.022*
C9	0.24576 (19)	0.43850 (19)	0.18264 (15)	0.0188 (3)
C10	0.2175 (2)	0.4733 (2)	−0.02788 (15)	0.0244 (4)

H10A	0.3176	0.5663	0.0132	0.029*
H10B	0.1363	0.5023	−0.0897	0.029*
C11	0.2686 (2)	0.3427 (2)	−0.09767 (18)	0.0325 (4)
H11A	0.315	0.3746	−0.1659	0.049*
H11B	0.1701	0.2496	−0.1356	0.049*
H11C	0.3541	0.3186	−0.0372	0.049*
C12	0.2467 (2)	0.1698 (2)	0.31142 (14)	0.0195 (3)
C13	0.2088 (2)	−0.1139 (2)	0.13307 (17)	0.0294 (4)
H13A	0.1576	−0.18	0.0448	0.044*
H13B	0.1628	−0.1673	0.1925	0.044*
H13C	0.3309	−0.0944	0.1545	0.044*
C14	0.4017 (3)	0.2120 (2)	0.56368 (16)	0.0317 (4)
H14A	0.4778	0.3092	0.5589	0.048*
H14B	0.4595	0.1723	0.6305	0.048*
H14C	0.3018	0.2324	0.5847	0.048*
N1	0.20693 (17)	0.56002 (17)	0.48823 (12)	0.0200 (3)
N2	0.23886 (17)	0.30580 (16)	0.35854 (12)	0.0200 (3)
O1	0.06584 (17)	0.61847 (16)	0.31231 (11)	0.0308 (3)
O2	0.39713 (14)	0.48975 (15)	0.20888 (11)	0.0265 (3)
O3	0.14030 (13)	0.42455 (14)	0.07059 (10)	0.0217 (3)
S1	0.16283 (5)	0.06980 (5)	0.14655 (4)	0.02388 (13)
S2	0.33924 (6)	0.06874 (5)	0.41135 (4)	0.02561 (14)
H1F	0.254 (2)	0.487 (2)	0.5037 (18)	0.031*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0190 (7)	0.0190 (9)	0.0168 (7)	0.0042 (6)	0.0079 (6)	0.0029 (6)
C2	0.0246 (8)	0.0205 (9)	0.0218 (8)	0.0075 (7)	0.0089 (7)	0.0064 (7)
C3	0.0335 (9)	0.0187 (9)	0.0300 (9)	0.0100 (7)	0.0155 (8)	0.0061 (7)
C4	0.0343 (9)	0.0227 (10)	0.0251 (9)	0.0037 (8)	0.0121 (8)	−0.0017 (7)
C5	0.0272 (9)	0.0317 (11)	0.0187 (8)	0.0059 (8)	0.0030 (7)	0.0024 (7)
C6	0.0243 (8)	0.0268 (10)	0.0220 (8)	0.0095 (7)	0.0061 (7)	0.0059 (7)
C7	0.0205 (7)	0.0190 (9)	0.0189 (7)	0.0062 (6)	0.0062 (7)	0.0044 (6)
C8	0.0210 (7)	0.0178 (8)	0.0165 (7)	0.0065 (6)	0.0035 (6)	0.0040 (6)
C9	0.0217 (8)	0.0162 (8)	0.0182 (7)	0.0080 (6)	0.0036 (7)	0.0025 (6)
C10	0.0272 (8)	0.0315 (10)	0.0191 (8)	0.0124 (7)	0.0075 (7)	0.0113 (7)
C11	0.0356 (10)	0.0377 (12)	0.0288 (9)	0.0133 (9)	0.0161 (8)	0.0086 (8)
C12	0.0212 (7)	0.0201 (9)	0.0177 (7)	0.0057 (6)	0.0062 (7)	0.0055 (6)
C13	0.0382 (10)	0.0196 (9)	0.0280 (9)	0.0107 (8)	0.0077 (8)	−0.0001 (7)
C14	0.0426 (10)	0.0306 (11)	0.0177 (8)	0.0121 (9)	−0.0001 (8)	0.0043 (7)
N1	0.0251 (7)	0.0197 (8)	0.0175 (6)	0.0116 (6)	0.0057 (6)	0.0040 (5)
N2	0.0243 (7)	0.0189 (7)	0.0173 (6)	0.0082 (6)	0.0048 (6)	0.0049 (5)
O1	0.0461 (7)	0.0291 (7)	0.0208 (6)	0.0229 (6)	0.0034 (6)	0.0061 (5)
O2	0.0202 (6)	0.0324 (8)	0.0245 (6)	0.0052 (5)	0.0029 (5)	0.0092 (5)
O3	0.0208 (6)	0.0300 (7)	0.0153 (5)	0.0094 (5)	0.0038 (5)	0.0072 (5)
S1	0.0304 (2)	0.0213 (2)	0.0173 (2)	0.00912 (18)	0.00318 (17)	0.00107 (16)
S2	0.0351 (3)	0.0212 (2)	0.0211 (2)	0.01201 (19)	0.00365 (19)	0.00657 (17)

Geometric parameters (Å, º)

C1—C6	1.392 (2)	C10—O3	1.4683 (19)
C1—C2	1.395 (2)	C10—C11	1.498 (3)
C1—N1	1.412 (2)	C10—H10A	0.99
C2—C3	1.390 (2)	C10—H10B	0.99
C2—H2	0.95	C11—H11A	0.98
C3—C4	1.384 (3)	C11—H11B	0.98
C3—H3	0.95	C11—H11C	0.98
C4—C5	1.386 (3)	C12—N2	1.273 (2)
C4—H4	0.95	C12—S2	1.7587 (17)
C5—C6	1.388 (2)	C12—S1	1.7678 (16)
C5—H5	0.95	C13—S1	1.8035 (19)
C6—H6	0.95	C13—H13A	0.98
C7—O1	1.2217 (19)	C13—H13B	0.98
C7—N1	1.347 (2)	C13—H13C	0.98
C7—C8	1.541 (2)	C14—S2	1.7968 (18)
C8—N2	1.461 (2)	C14—H14A	0.98
C8—C9	1.532 (2)	C14—H14B	0.98
C8—H8	1	C14—H14C	0.98
C9—O2	1.2075 (19)	N1—H1F	0.889 (15)
C9—O3	1.3292 (18)		
C6—C1—C2	120.11 (15)	C11—C10—H10A	109.6
C6—C1—N1	116.63 (15)	O3—C10—H10B	109.6
C2—C1—N1	123.25 (14)	C11—C10—H10B	109.6
C3—C2—C1	118.97 (16)	H10A—C10—H10B	108.2
C3—C2—H2	120.5	C10—C11—H11A	109.5
C1—C2—H2	120.5	C10—C11—H11B	109.5
C4—C3—C2	121.22 (17)	H11A—C11—H11B	109.5
C4—C3—H3	119.4	C10—C11—H11C	109.5
C2—C3—H3	119.4	H11A—C11—H11C	109.5
C3—C4—C5	119.36 (16)	H11B—C11—H11C	109.5
C3—C4—H4	120.3	N2—C12—S2	120.47 (12)
C5—C4—H4	120.3	N2—C12—S1	123.28 (12)
C4—C5—C6	120.39 (16)	S2—C12—S1	116.23 (10)
C4—C5—H5	119.8	S1—C13—H13A	109.5
C6—C5—H5	119.8	S1—C13—H13B	109.5
C5—C6—C1	119.94 (17)	H13A—C13—H13B	109.5
C5—C6—H6	120	S1—C13—H13C	109.5
C1—C6—H6	120	H13A—C13—H13C	109.5
O1—C7—N1	126.13 (16)	H13B—C13—H13C	109.5
O1—C7—C8	120.39 (14)	S2—C14—H14A	109.5
N1—C7—C8	113.48 (14)	S2—C14—H14B	109.5
N2—C8—C9	112.30 (13)	H14A—C14—H14B	109.5
N2—C8—C7	110.24 (12)	S2—C14—H14C	109.5
C9—C8—C7	106.50 (13)	H14A—C14—H14C	109.5
N2—C8—H8	109.2	H14B—C14—H14C	109.5

C9—C8—H8	109.2	C7—N1—C1	129.37 (14)
C7—C8—H8	109.2	C7—N1—H1F	111.8 (13)
O2—C9—O3	125.06 (15)	C1—N1—H1F	118.7 (13)
O2—C9—C8	123.37 (14)	C12—N2—C8	120.84 (13)
O3—C9—C8	111.54 (13)	C9—O3—C10	116.15 (12)
O3—C10—C11	110.09 (15)	C12—S1—C13	104.78 (8)
O3—C10—H10A	109.6	C12—S2—C14	99.96 (8)
C6—C1—C2—C3	0.3 (2)	O1—C7—N1—C1	−2.9 (3)
N1—C1—C2—C3	−179.69 (15)	C8—C7—N1—C1	176.35 (15)
C1—C2—C3—C4	−0.1 (3)	C6—C1—N1—C7	−171.05 (16)
C2—C3—C4—C5	−0.1 (3)	C2—C1—N1—C7	8.9 (3)
C3—C4—C5—C6	0.0 (3)	S2—C12—N2—C8	−175.45 (11)
C4—C5—C6—C1	0.2 (3)	S1—C12—N2—C8	2.8 (2)
C2—C1—C6—C5	−0.4 (2)	C9—C8—N2—C12	−70.50 (19)
N1—C1—C6—C5	179.60 (15)	C7—C8—N2—C12	170.92 (14)
O1—C7—C8—N2	−179.82 (15)	O2—C9—O3—C10	1.2 (2)
N1—C7—C8—N2	0.92 (19)	C8—C9—O3—C10	179.46 (13)
O1—C7—C8—C9	58.11 (19)	C11—C10—O3—C9	83.60 (18)
N1—C7—C8—C9	−121.15 (14)	N2—C12—S1—C13	179.81 (14)
N2—C8—C9—O2	−38.3 (2)	S2—C12—S1—C13	−1.86 (12)
C7—C8—C9—O2	82.41 (19)	N2—C12—S2—C14	−1.14 (16)
N2—C8—C9—O3	143.40 (13)	S1—C12—S2—C14	−179.52 (10)
C7—C8—C9—O3	−95.84 (15)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*F*···N2	0.889 (15)	2.019 (18)	2.586 (2)	120.5 (15)
C2—H2···O1	0.95	2.33	2.932 (2)	121
C6—H6···O2^{i}	0.95	2.4	3.295 (2)	156
C10—H10*B*···O1^{ii}	0.99	2.53	3.340 (2)	138
C10—H10*B*···O3^{ii}	0.99	2.65	3.377 (2)	131
C11—H11*A*···O2^{iii}	0.98	2.64	3.465 (2)	141
C13—H13*B*···O1^{iv}	0.98	2.63	3.579 (2)	162

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