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(*Z*)-2-(Dimethylamino)-5-(3,4,5-trimethoxybenzylidene)-1,3-thiazolidin-4-one

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.002 Å
R factor = 0.041
wR factor = 0.106
Data-to-parameter ratio = 16.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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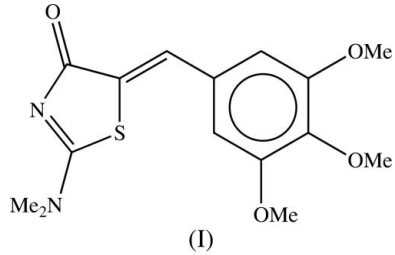
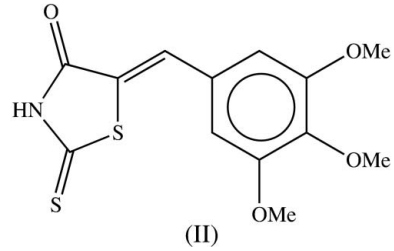
In the title compound, $C_{15}H_{18}N_2O_4S$, there is a very wide C—C—C angle [130.72 (16)°] at the methine C atom linking the two rings. A single C—H···O hydrogen bond links pairs of molecules into dimers around a twofold axis.

Comment

We have recently described (Delgado *et al.*, 2005, 2006) the structures of a range of (*Z*)-5-benzylidene-2-thioxothiazolidin-4-ones that had originally been synthesized both as potential intermediates for the synthesis of fused heterocyclic systems, and as potential antifungal agents (Sortino *et al.*, 2007). As part of an effort to diversify the substituents, particularly in respect of the antifungal activity, we now report the structure of the related analogue (I) (Fig. 1), which was obtained by reaction of dimethylamine with the previously described (Delgado *et al.*, 2006) (*Z*)-5-(3,4,5-trimethoxybenzylidene)-2-thioxothiazolidin-4-one, (II).



(I)



(II)

As with all of the (*Z*)-5-benzylidene-2-thioxothiazolidin-4-ones, the molecular skeleton of (I) is almost planar, as shown by the key torsion angles, and it exhibits a very wide C—C—C angle at the methine C atom linking the two rings (Table 1). The exocyclic bond angles at atoms C5 and C51 are consistent with a repulsive intramolecular interaction between S1 and H56 (Fig. 1). The conformation of the methoxy groups, and the pattern of the exocyclic C—C—O bond angles at C53, C54 and C55 closely follows the behaviour observed in (II) (Delgado *et al.*, 2006).

A single, almost linear C—H···O hydrogen bond (Table 2) links a pair of molecules into an $R_2^2(14)$ (Bernstein *et al.*, 1995)

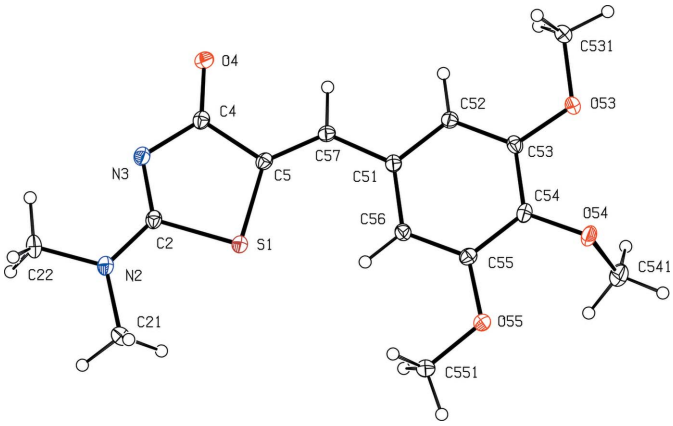


Figure 1
The molecular structure of compound (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

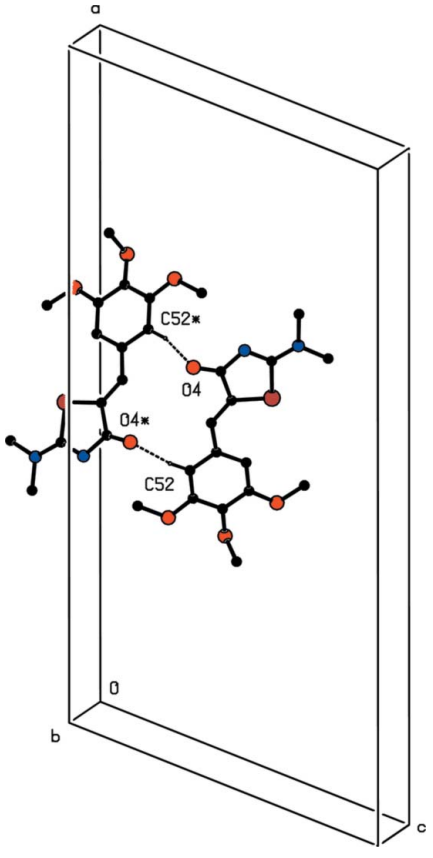


Figure 2
Part of the crystal structure of compound (I) showing the formation of a cyclic hydrogen-bonded (dashed lines) dimer. For the sake of clarity, the H atoms not involved in the motif shown have been omitted. The atoms marked with an asterisk (*) are at the symmetry position $(1-x, y, \frac{1}{2}-z)$.

dimer lying across a twofold rotation axis and quite sharply folded across the intra-ring O···O vectors. There are four dimers of this type in each unit cell. Fairly short contacts occur between the heterocyclic ring of the molecule at (x, y, z), which is part of a hydrogen-bonded dimer across the axis $(\frac{1}{2}, y, \frac{1}{4})$ and the aryl ring of the molecule at $(1-x, 1-y, 1-z)$,

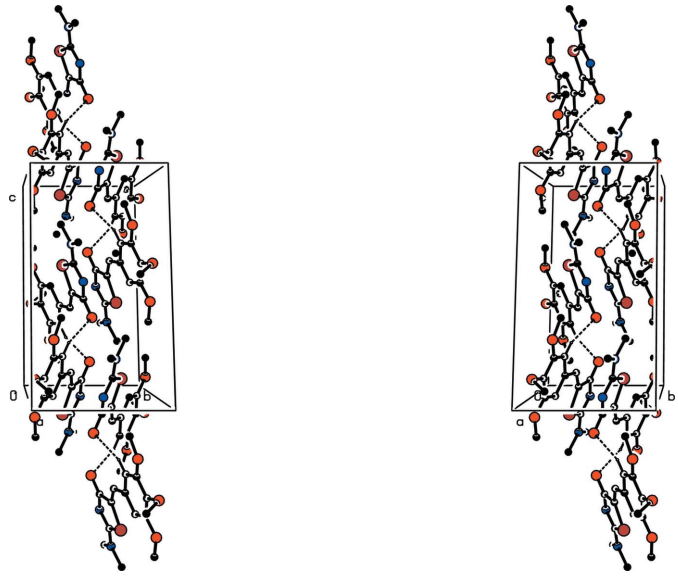


Figure 3
A stereoview of part of the crystal structure of compound (I), showing a chain of hydrogen-bonded (dashed lines) dimers along [001]. For the sake of clarity, the H atoms not involved in the motif shown have been omitted.

which forms part of a hydrogen-bonded dimer across $(\frac{1}{2}, -y, \frac{3}{4})$. Hence the dimers aligned along [001] form a series of short contacts (Fig. 3), with an interplanar angle between adjacent heterocyclic and aryl rings of 3.9 (2)°, a ring-centroid separation of 3.492 (2) Å, and an interplanar spacing of *ca* 3.33 Å. However, since the thiazolidin-4-one ring exhibits no aromatic type delocalization, it is unlikely that these contacts are other than adventitious, associated with little or no direction-specific interaction energy between adjacent dimers.

Experimental

A solution of (II) (1 mmol) and dimethylamine (0.5 mmol) in *N*,*N*-dimethylformamide (2 ml) was heated under reflux for 6 h. The mixture was cooled to ambient temperature, and the resulting precipitate was collected by filtration and washed with ethanol; crystallization from *N*,*N*-dimethylformamide provided yellow crystals suitable for single-crystal X-ray diffraction; yield 64%, m. p. 478–479 K.

Crystal data

$C_{15}H_{18}N_2O_4S$
$M_r = 322.37$
Monoclinic, $C2/c$
$a = 29.259$ (6) Å
$b = 7.6410$ (15) Å
$c = 14.336$ (3) Å
$\beta = 110.59$ (3)°
$V = 3000.3$ (11) Å^3
$Z = 8$
$D_x = 1.427$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.24$ mm^{-1}
$T = 120$ (2) K
Block, yellow
0.48 × 0.25 × 0.20 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{min} = 0.904$, $T_{max} = 0.954$
34966 measured reflections
3433 independent reflections
2798 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$
$\theta_{max} = 27.5°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0405P)^2 + 5.225P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.041$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.106$	$\Delta\rho_{max} = 0.31$ e Å^{-3}
$S = 1.11$	$\Delta\rho_{min} = -0.38$ e Å^{-3}
3433 reflections	
204 parameters	
H-atom parameters constrained	

Table 1
Selected bond and torsion angles (°).

C5—C57—C51	130.72 (16)	O53—C53—C54	115.90 (15)
S1—C5—C57	129.59 (14)	C54—O54—C541	113.56 (14)
C4—C5—C57	121.69 (15)	O54—C54—C53	119.39 (15)
C52—C51—C57	117.02 (15)	O54—C54—C55	121.02 (15)
C56—C51—C57	123.21 (15)	C55—O55—C551	116.47 (13)
C53—O53—C531	116.67 (13)	O55—C55—C54	115.78 (15)
O53—C53—C52	123.97 (15)	O55—C55—C56	123.59 (16)
S1—C2—N2—C21	−0.9 (2)	C52—C53—O53—C531	6.9 (2)
S1—C2—N2—C22	173.48 (14)	C53—C54—O54—C541	−105.43 (19)
C4—C5—C57—C51	178.74 (16)	C56—C55—O55—C551	3.5 (2)
C5—C57—C51—C52	−177.26 (17)		

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

D—H···A	D—H	H···A	D···A	D—H···A
C52—H52···O4^{i}	0.95	2.30	3.216 (2)	162

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

All H atoms were located in difference maps and then treated as riding atoms with C—H distances 0.95 Å (aromatic and methine) or 0.98 Å (methyl), and with $U_{iso}(H) = kU_{eq}(C)$, where $k = 1.5$ for the methyl groups and 1.2 for all other H atoms.

Data collection: *COLLECT* (Hooft, 1999); cell refinement: *DIRAX/LSQ* (Duisenberg *et al.*, 2000); data reduction: *EVALCCD* (Duisenberg *et al.*, 2003); program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *OSCAIL* (McArdle, 2003) and *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PRPKAPPA* (Ferguson, 1999).

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$M_r = 322.37$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 29.259\ (6)$ Å
$b = 7.6410\ (15)$ Å
$c = 14.336\ (3)$ Å
$\beta = 110.59\ (3)°$
$V = 3000.3\ (11)$ Å^3
$Z = 8$
$F(000) = 1360$
$D_x = 1.427$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3433 reflections
$\theta = 3.8–27.5°$
$\mu = 0.24$ mm^{-1}
$T = 120$ K
Plate, yellow
0.48 × 0.25 × 0.20 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
Radiation source: Bruker-Nonius FR591 rotating anode
Graphite monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
$T_{min} = 0.904$, $T_{max} = 0.954$
34966 measured reflections
3433 independent reflections
2798 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.8°$
$h = -37\rightarrow37$
$k = -9\rightarrow9$
$l = -18\rightarrow18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.106$
$S = 1.11$
3433 reflections
204 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
$w = 1/[\sigma^2(F_o^2) + (0.0405P)^2 + 5.225P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.38$ e Å^{-3}

Special details

Experimental. MS (EI, 30 eV) *m*/*z* (%) 322 (37, M^+), 224 (100), 209 (76), 181 (12), 69 (9).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.563871 (15)	0.27949 (6)	0.58438 (3)	0.01972 (12)
C2	0.62209 (6)	0.3569 (2)	0.59098 (13)	0.0197 (3)
N2	0.65949 (5)	0.3382 (2)	0.67603 (11)	0.0224 (3)
C21	0.65416 (7)	0.2587 (3)	0.76418 (14)	0.0278 (4)
C22	0.70897 (7)	0.3826 (3)	0.68225 (15)	0.0312 (4)
N3	0.62541 (5)	0.4299 (2)	0.51078 (11)	0.0210 (3)
C4	0.58079 (6)	0.4360 (2)	0.43445 (13)	0.0197 (3)
O4	0.57382 (5)	0.50106 (17)	0.35237 (9)	0.0237 (3)
C5	0.54014 (6)	0.3528 (2)	0.46079 (12)	0.0186 (3)
C57	0.49437 (6)	0.3411 (2)	0.39417 (12)	0.0183 (3)
C51	0.45034 (6)	0.2642 (2)	0.40300 (12)	0.0182 (3)
C52	0.40797 (6)	0.2660 (2)	0.31737 (12)	0.0186 (3)
C53	0.36473 (6)	0.1951 (2)	0.32008 (12)	0.0192 (3)
O53	0.32162 (4)	0.19222 (18)	0.23984 (9)	0.0238 (3)
C531	0.32375 (7)	0.2495 (3)	0.14624 (13)	0.0263 (4)
C54	0.36312 (6)	0.1219 (2)	0.40826 (13)	0.0199 (3)
O54	0.32059 (4)	0.04416 (18)	0.40839 (10)	0.0262 (3)
C541	0.29455 (7)	0.1465 (3)	0.45608 (16)	0.0347 (5)
C55	0.40532 (6)	0.1223 (2)	0.49410 (12)	0.0197 (3)
O55	0.40052 (4)	0.04945 (18)	0.57703 (9)	0.0251 (3)
C551	0.44261 (7)	0.0564 (3)	0.66656 (13)	0.0245 (4)
C56	0.44876 (6)	0.1923 (2)	0.49177 (13)	0.0198 (3)
H21A	0.6549	0.1310	0.7587	0.042*
H21B	0.6230	0.2949	0.7693	0.042*
H21C	0.6810	0.2969	0.8237	0.042*
H22A	0.7083	0.4260	0.6175	0.047*
H22B	0.7297	0.2782	0.7006	0.047*
H22C	0.7221	0.4735	0.7328	0.047*
H57	0.4900	0.3912	0.3309	0.022*
H52	0.4089	0.3160	0.2574	0.022*
H53A	0.3462	0.1743	0.1274	0.039*
H53B	0.3354	0.3707	0.1523	0.039*
H53C	0.2911	0.2427	0.0950	0.039*
H54A	0.2663	0.0801	0.4586	0.052*
H54B	0.2833	0.2549	0.4185	0.052*
H54C	0.3161	0.1749	0.5240	0.052*
H55A	0.4524	0.1786	0.6825	0.037*
H55B	0.4694	−0.0088	0.6569	0.037*
H55C	0.4347	0.0042	0.7215	0.037*
H56	0.4772	0.1914	0.5500	0.024*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0165 (2)	0.0226 (2)	0.0202 (2)	−0.00036 (16)	0.00663 (16)	0.00106 (16)

C2	0.0171 (8)	0.0204 (8)	0.0226 (8)	0.0004 (6)	0.0082 (7)	−0.0028 (7)
N2	0.0166 (7)	0.0261 (8)	0.0245 (8)	0.0010 (6)	0.0071 (6)	0.0008 (6)
C21	0.0238 (9)	0.0353 (10)	0.0213 (9)	0.0002 (8)	0.0041 (7)	0.0023 (8)
C22	0.0154 (8)	0.0424 (12)	0.0333 (10)	−0.0017 (8)	0.0052 (7)	0.0004 (9)
N3	0.0176 (7)	0.0229 (7)	0.0234 (7)	−0.0007 (6)	0.0085 (6)	−0.0014 (6)
C4	0.0189 (8)	0.0194 (8)	0.0225 (8)	−0.0003 (6)	0.0094 (7)	−0.0042 (7)
O4	0.0249 (6)	0.0275 (7)	0.0209 (6)	−0.0019 (5)	0.0108 (5)	−0.0002 (5)
C5	0.0191 (8)	0.0185 (8)	0.0206 (8)	0.0001 (6)	0.0099 (7)	−0.0023 (7)
C57	0.0198 (8)	0.0192 (8)	0.0177 (8)	0.0008 (6)	0.0086 (6)	−0.0030 (6)
C51	0.0172 (8)	0.0190 (8)	0.0190 (8)	0.0000 (6)	0.0072 (6)	−0.0045 (6)
C52	0.0192 (8)	0.0194 (8)	0.0181 (8)	−0.0010 (6)	0.0076 (7)	−0.0029 (6)
C53	0.0165 (8)	0.0211 (8)	0.0186 (8)	0.0004 (6)	0.0042 (6)	−0.0043 (6)
O53	0.0156 (6)	0.0352 (7)	0.0186 (6)	−0.0014 (5)	0.0034 (5)	−0.0001 (5)
C531	0.0197 (8)	0.0377 (11)	0.0191 (8)	−0.0007 (8)	0.0040 (7)	0.0007 (8)
C54	0.0167 (8)	0.0195 (8)	0.0251 (9)	−0.0023 (6)	0.0093 (7)	−0.0034 (7)
O54	0.0190 (6)	0.0325 (7)	0.0294 (7)	−0.0079 (5)	0.0114 (5)	−0.0031 (6)
C541	0.0234 (9)	0.0484 (13)	0.0356 (11)	−0.0008 (9)	0.0146 (8)	−0.0032 (10)
C55	0.0215 (8)	0.0189 (8)	0.0206 (8)	−0.0006 (7)	0.0096 (7)	−0.0010 (7)
O55	0.0211 (6)	0.0329 (7)	0.0208 (6)	−0.0052 (5)	0.0069 (5)	0.0050 (5)
C551	0.0241 (9)	0.0280 (9)	0.0210 (9)	−0.0011 (7)	0.0076 (7)	0.0035 (7)
C56	0.0178 (8)	0.0228 (9)	0.0184 (8)	−0.0008 (6)	0.0058 (6)	−0.0025 (7)

Geometric parameters (Å, º)

S1—C5	1.7522 (18)	C52—H52	0.95
S1—C2	1.7740 (17)	C53—O53	1.376 (2)
C2—N3	1.312 (2)	C53—C54	1.398 (2)
C2—N2	1.329 (2)	O53—C531	1.433 (2)
N2—C22	1.459 (2)	C531—H53A	0.98
N2—C21	1.459 (2)	C531—H53B	0.98
C21—H21A	0.98	C531—H53C	0.98
C21—H21B	0.98	C54—O54	1.379 (2)
C21—H21C	0.98	C54—C55	1.404 (2)
C22—H22A	0.98	O54—C541	1.423 (2)
C22—H22B	0.98	C541—H54A	0.98
C22—H22C	0.98	C541—H54B	0.98
N3—C4	1.378 (2)	C541—H54C	0.98
C4—O4	1.227 (2)	C55—O55	1.364 (2)
C4—C5	1.509 (2)	C55—C56	1.390 (2)
C5—C57	1.347 (2)	O55—C551	1.434 (2)
C57—C51	1.461 (2)	C551—H55A	0.98
C57—H57	0.95	C551—H55B	0.98
C51—C56	1.402 (2)	C551—H55C	0.98
C51—C52	1.405 (2)	C56—H56	0.95
C52—C53	1.389 (2)		
C5—S1—C2	88.79 (8)	C51—C52—H52	119.9
N3—C2—N2	123.98 (16)	C52—C53—C54	120.13 (16)

N3—C2—S1	117.44 (13)	C53—O53—C531	116.67 (13)
N2—C2—S1	118.58 (13)	O53—C53—C52	123.97 (15)
C2—N2—C22	120.68 (15)	O53—C53—C54	115.90 (15)
C2—N2—C21	122.36 (15)	O53—C531—H53A	109.5
C22—N2—C21	116.73 (15)	O53—C531—H53B	109.5
N2—C21—H21A	109.5	H53A—C531—H53B	109.5
N2—C21—H21B	109.5	O53—C531—H53C	109.5
H21A—C21—H21B	109.5	H53A—C531—H53C	109.5
N2—C21—H21C	109.5	H53B—C531—H53C	109.5
H21A—C21—H21C	109.5	C53—C54—C55	119.53 (15)
H21B—C21—H21C	109.5	C54—O54—C541	113.56 (14)
N2—C22—H22A	109.5	O54—C54—C53	119.39 (15)
N2—C22—H22B	109.5	O54—C54—C55	121.02 (15)
H22A—C22—H22B	109.5	O54—C541—H54A	109.5
N2—C22—H22C	109.5	O54—C541—H54B	109.5
H22A—C22—H22C	109.5	H54A—C541—H54B	109.5
H22B—C22—H22C	109.5	O54—C541—H54C	109.5
C2—N3—C4	111.62 (15)	H54A—C541—H54C	109.5
O4—C4—N3	124.51 (16)	H54B—C541—H54C	109.5
O4—C4—C5	122.08 (16)	C56—C55—C54	120.63 (16)
N3—C4—C5	113.41 (15)	C55—O55—C551	116.47 (13)
C4—C5—S1	108.71 (12)	O55—C55—C54	115.78 (15)
C5—C57—C51	130.72 (16)	O55—C55—C56	123.59 (16)
S1—C5—C57	129.59 (14)	O55—C551—H55A	109.5
C4—C5—C57	121.69 (15)	O55—C551—H55B	109.5
C52—C51—C57	117.02 (15)	H55A—C551—H55B	109.5
C56—C51—C57	123.21 (15)	O55—C551—H55C	109.5
C5—C57—H57	114.6	H55A—C551—H55C	109.5
C51—C57—H57	114.6	H55B—C551—H55C	109.5
C56—C51—C52	119.77 (15)	C55—C56—C51	119.67 (16)
C53—C52—C51	120.27 (16)	C55—C56—H56	120.2
C53—C52—H52	119.9	C51—C56—H56	120.2

C5—S1—C2—N3	−0.45 (14)	C57—C51—C52—C53	179.93 (15)
C5—S1—C2—N2	179.43 (15)	C51—C52—C53—O53	179.70 (15)
N3—C2—N2—C22	−6.6 (3)	C51—C52—C53—C54	0.2 (3)
N3—C2—N2—C21	179.01 (17)	C52—C53—O53—C531	6.9 (2)
S1—C2—N2—C21	−0.9 (2)	C54—C53—O53—C531	−173.58 (15)
S1—C2—N2—C22	173.48 (14)	O53—C53—C54—O54	3.7 (2)
N2—C2—N3—C4	−178.42 (16)	C52—C53—C54—O54	−176.76 (15)
S1—C2—N3—C4	1.5 (2)	O53—C53—C54—C55	−178.91 (15)
C2—N3—C4—O4	178.41 (16)	C52—C53—C54—C55	0.6 (3)
C2—N3—C4—C5	−1.9 (2)	C53—C54—O54—C541	−105.43 (19)
O4—C4—C5—C57	2.1 (3)	C55—C54—O54—C541	77.2 (2)
N3—C4—C5—C57	−177.59 (15)	O54—C54—C55—O55	−3.1 (2)
O4—C4—C5—S1	−178.75 (14)	C53—C54—C55—O55	179.57 (15)
N3—C4—C5—S1	1.55 (18)	O54—C54—C55—C56	176.40 (15)
C2—S1—C5—C57	178.44 (17)	C53—C54—C55—C56	−0.9 (3)

C2—S1—C5—C4	−0.61 (12)	C56—C55—O55—C551	3.5 (2)
C4—C5—C57—C51	178.74 (16)	C54—C55—O55—C551	−177.05 (15)
S1—C5—C57—C51	−0.2 (3)	O55—C55—C56—C51	179.87 (15)
C5—C57—C51—C56	3.4 (3)	C54—C55—C56—C51	0.4 (3)
C5—C57—C51—C52	−177.26 (17)	C52—C51—C56—C55	0.4 (2)
C56—C51—C52—C53	−0.7 (2)	C57—C51—C56—C55	179.72 (16)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C52—H52···O4^{i}	0.95	2.30	3.216 (2)	162

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