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2-(4-Amino-5-thioxo-4,5-dihydro-1*H*-1,2,4-triazol-3-ylmethyl)isoindoline-1,3-dione

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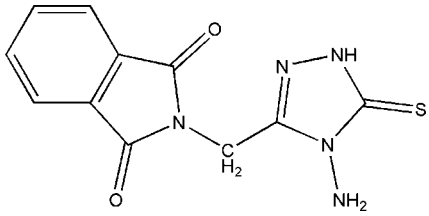
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.029; wR factor = 0.070; data-to-parameter ratio = 12.8.

The title compound, $C_{11}H_9N_5O_2S$, was synthesized from *N*-phthaloylglycine and thiocarbohydrazide by the fusion method. This is the first report of a triazole derivative of *N*-phthaloylglycine. The title compound exists in the thione form. The molecule is non-planar, with a dihedral angle between the isoindoline ring system and the triazole ring system of 82.24 (5)°. The crystal structure is stabilized by intermolecular hydrogen bonding linking the molecules into a three-dimensional network.

Related literature

For related literature, see: Allen *et al.* (1987); Antunes *et al.* (1998); Barooah *et al.* (2006*a*,*b*); Brana & Ramos (2001); Chandrasekhar *et al.* (1999); Eugenio, *et al.* (2004); Görner *et al.* (2002); Khan & Ismail (2002); Matijević-Sosa & Cvetnić (2005); Neto *et al.* (1993); Ng (1992); Shariat & Abdollahi (2004); Wang *et al.* (1998); Xu *et al.* (2005), Zhang *et al.* (2004).



Experimental

Crystal data

$C_{11}H_9N_5O_2S$
M_r = 275.29
Orthorhombic, $Pna2_1$
a = 5.1961 (11) Å
b = 19.952 (4) Å
c = 11.336 (3) Å
V = 1175.2 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.28 mm^{-1}
T = 100 (2) K
0.60 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker 2001)
T_{min} = 0.849, T_{max} = 0.946
6288 measured reflections
2361 independent reflections
2281 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.069
S = 1.04
2361 reflections
184 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Absolute structure: Flack (1983), with 1091 Friedel pairs
Flack parameter: −0.04 (6)

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

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5*M*···O2^{i}	0.92 (2)	2.29 (2)	3.151 (2)	155.6 (19)
N5—H5*N*···S1^{ii}	0.83 (2)	2.60 (2)	3.430 (2)	177.4 (18)
N3—H3*N*···O1^{iii}	0.84 (2)	1.98 (2)	2.811 (2)	169 (2)

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RN2038).

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supporting information

Acta Cryst. (2008). E**64**, o476–o477 [doi:10.1107/S1600536808001189]

2-(4-Amino-5-thioxo-4,5-dihydro-1*H*-1,2,4-triazol-3-ylmethyl)isoindoline-1,3-dione

Uzma Yunus, Mohammad Kalim Tahir, Moazzam Hussain Bhatti, Naveeda Yousaf and Madeleine Helliwell

S1. Comment

Phthalimide and its derivatives such as *N*-phthaloylamino acids are used for the synthesis of peptide bonds in solid phase synthesis (Eugenio *et al.*, 2004; Chandrasekhar *et al.*, 1999). Such phthalimide derivatives undergo photochemical reactions such as photochemical decomposition and decarboxylation (Görner *et al.*, 2002). Moreover *N*-phthaloylamino acids and their derivatives possess a wide range of biological activities such as hypolipidemic (Neto *et al.*, 1993) analgesic (Antunes *et al.*, 1998) antimicrobial (Matijević-Sosa & Cvetnić, 2005) and DNA cleaving abilities (Brana & Ramos, 2001). Among the *N*-phthaloylamino acids, N-phthaloylglycine has been the most widely studied. Such studies include cleavage of N-phthaloylglycine with various amines (Khan & Ismail, 2002), metal complexes with interesting supramolecular structures (Barooah *et al.*, 2006*b*) and adduct formation of N-phthaloylglycine with various aromatic amines and hydroxyl-aromatics (Barooah *et al.*, 2006*a*). The heterocyclic derivatives of N-phthaloylglycine are also reported in literature such as oxadiazole (Antunes *et al.*, 1998) and benzoxazinone (Shariat & Abdollahi, 2004). Keeping in view the importance of structural and biological aspects of *N*-phthaloylamino acids, the present work is aiming to incorporate 1,2,4-triazole ring with N-phthaloylglycine moiety. To the best of our knowledge this is the first crystal structure report on the 1,2,4-triazole derivative of N-phthaloylglycine.

The crystallographic analysis demonstrates that the title compound (I) exists as the thione form rather than the thiol as shown in scheme 1 and Fig. 1. The triazole ring is essentially planar. The C?S bond length [1.6758 (19) Å] is slightly longer than a pure double bond [1.61 Å] (Allen *et al.*, 1987) and is comparable with analogous compounds (Zhang *et al.*, 2004; Xu *et al.*,2005). The CN bond distances of the triazole ring are in the range 1.297 (2)–1.374 (2) Å in which the N4—C10 bond shows double bond character. The other CN bonds have values intermediate between those expected for single and double C—N bonds [1.47 and 1.27 Å respectively (Allen *et al.*, 1987)] among which the N2—C11 bond length is slightly longer than that of N3—C11 (Wang *et al.*, 1998). The NN bond lengths and all bond angles in triazole ring show no significant difference when compared to analogous compounds.

The phthalimide is also planar and all bond lengths and angles in the phthalimide ring are within normal ranges (Ng, 1992). The dihedral angle between the isoindoline and triazole ring systems is 82.24 (5)°, indicating the nonplanarity of the molecule as a whole.

The molecules are linked into pairs by the intermolecular hydrogen bond N5—H5N···S1 (symmetry equivalent $x + 1/2$, $-y + 3/2$, z) and then into sheets by the N3—H3N···O1 ($-x$, $-y + 1$, $z - 1/2$) contact, and finally into a three-dimensional network by the hydrogen bonds N5—H5M···O2 (symmetry equivalent $x - 1$, y, z) linking the sheets in the a direction.

S2. Experimental

The title compound (I) was synthesized by the reaction of N-phthaloylglycine and thiocarbohydrazide by the fusion method. A mixture of N-phthaloylglycine (0.01 mol) and thiocarbohydrazide (0.01 mol) contained in a round bottom flask was heated until the contents melted. The mixture was kept at this temperature for 25–30 min. after cooling to room temperature the mixture was triturated with methanol and the solid obtained was filtered, washed with methanol and recrystallized from a mixture (1:1) of ethanol and acetonitrile to obtain suitable crystals for *x*-ray analysis.

S3. Refinement

H atoms bonded to C were included in calculated positions with C—H distances ranging from 0.95–0.99 Å and U_{eq} 1.2 times those of the parent atoms; those bonded to N were found by difference Fourier techniques and refined isotropically. The absolute configuration was determined by refinement of the Flack parameter.

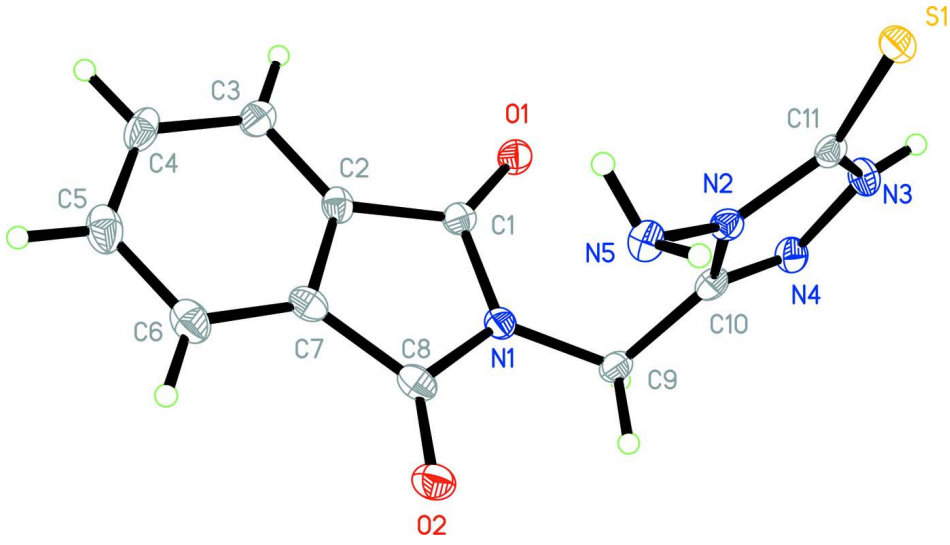

Figure 1

Plot of the title compound with ellipsoids drawn at the 50% probability level.

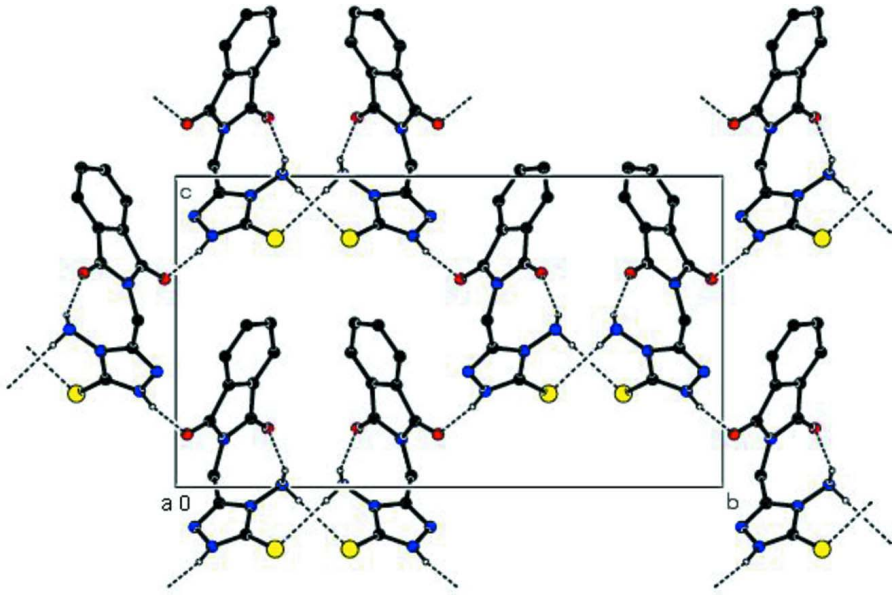

Figure 2

Packing of the title compound viewed down a, showing hydrogen bonding contacts with dashed lines.

2-(4-Amino-5-thioxo-4,5-dihydro-1*H*-1,2,4-triazol-3- ylmethyl)isoindoline-1,3-dione

Crystal data

$C_{11}H_9N_5O_2S$
$M_r = 275.29$
Orthorhombic, $Pna2_1$
Hall symbol: P2c-2n
$a = 5.1961$ (11) Å
$b = 19.952$ (4) Å
$c = 11.336$ (3) Å
$V = 1175.2$ (4) Å^3
$Z = 4$
$F(000) = 568$
$D_x = 1.556$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 934 reflections
$\theta = 3.6$–$26.4°$
$\mu = 0.28$ mm^{-1}
$T = 100$ K
Plate, colourless
0.60 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker 2001)
$T_{min} = 0.849$, $T_{max} = 0.946$
6288 measured reflections
2361 independent reflections
2281 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 26.4°$, $\theta_{min} = 2.0°$
$h = -6 \rightarrow 6$
$k = -24 \rightarrow 17$
$l = -14 \rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.069$
$S = 1.04$
2361 reflections
184 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0413P)^2 + 0.1704P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}
Absolute structure: Flack (1983), 1091 Friedel pairs
Absolute structure parameter: −0.04 (6)

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	−0.14861 (8)	0.68164 (2)	0.30015 (4)	0.01625 (11)
O1	0.1683 (2)	0.52047 (6)	0.66973 (11)	0.0180 (3)
O2	0.8375 (3)	0.66831 (7)	0.68855 (12)	0.0214 (3)
N1	0.5265 (3)	0.58747 (7)	0.65527 (13)	0.0147 (3)
N2	0.2503 (3)	0.63673 (7)	0.43781 (13)	0.0130 (3)
N3	0.1312 (3)	0.56622 (7)	0.30883 (15)	0.0158 (3)
H3N	0.051 (5)	0.5428 (11)	0.259 (2)	0.025 (6)*
N4	0.3250 (3)	0.53474 (8)	0.37168 (15)	0.0166 (3)
N5	0.2864 (3)	0.69419 (8)	0.50736 (16)	0.0154 (3)
H5M	0.141 (4)	0.6996 (11)	0.553 (2)	0.018 (6)*
H5N	0.297 (4)	0.7244 (11)	0.4569 (19)	0.012 (5)*
C1	0.3120 (3)	0.56238 (9)	0.71243 (16)	0.0150 (4)
C2	0.3011 (4)	0.59671 (9)	0.82861 (14)	0.0152 (4)
C3	0.1294 (4)	0.59041 (10)	0.92077 (16)	0.0182 (4)
H3	−0.0128	0.5606	0.9163	0.022*
C4	0.1732 (4)	0.62951 (10)	1.02058 (17)	0.0214 (4)
H4	0.0574	0.6265	1.0852	0.026*
C5	0.3824 (4)	0.67281 (10)	1.02788 (19)	0.0230 (5)
H5	0.4097	0.6980	1.0979	0.028*
C6	0.5528 (4)	0.67960 (9)	0.93312 (18)	0.0211 (4)
H6	0.6953	0.7093	0.9370	0.025*
C7	0.5063 (4)	0.64151 (9)	0.83394 (16)	0.0165 (4)
C8	0.6511 (3)	0.63748 (9)	0.72124 (18)	0.0176 (4)
C9	0.6033 (3)	0.56940 (10)	0.53675 (16)	0.0154 (4)
H9A	0.6560	0.5217	0.5358	0.018*
H9B	0.7544	0.5967	0.5138	0.018*
C10	0.3944 (3)	0.57960 (9)	0.44821 (17)	0.0147 (4)
C11	0.0778 (4)	0.62815 (9)	0.34723 (15)	0.0138 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0147 (2)	0.0187 (2)	0.0154 (2)	0.00169 (17)	−0.0019 (2)	−0.0004 (2)
O1	0.0184 (7)	0.0189 (6)	0.0168 (7)	−0.0046 (5)	0.0012 (5)	0.0002 (5)
O2	0.0170 (7)	0.0237 (7)	0.0234 (8)	−0.0047 (6)	−0.0012 (6)	0.0008 (6)
N1	0.0137 (8)	0.0169 (7)	0.0135 (8)	−0.0017 (6)	−0.0014 (6)	0.0016 (6)
N2	0.0128 (7)	0.0125 (7)	0.0136 (7)	−0.0016 (6)	0.0011 (6)	−0.0007 (6)
N3	0.0188 (7)	0.0143 (7)	0.0142 (8)	−0.0003 (6)	−0.0030 (7)	−0.0020 (7)
N4	0.0180 (8)	0.0166 (7)	0.0153 (8)	−0.0001 (6)	−0.0003 (6)	0.0009 (6)
N5	0.0194 (8)	0.0115 (7)	0.0153 (8)	−0.0002 (6)	0.0011 (7)	−0.0010 (6)
C1	0.0143 (9)	0.0160 (9)	0.0147 (9)	0.0023 (7)	−0.0003 (7)	0.0046 (7)
C2	0.0174 (9)	0.0145 (8)	0.0137 (9)	0.0034 (7)	−0.0024 (7)	0.0011 (7)
C3	0.0185 (9)	0.0198 (10)	0.0162 (10)	0.0043 (8)	0.0013 (7)	0.0038 (8)
C4	0.0258 (10)	0.0256 (11)	0.0130 (10)	0.0101 (8)	0.0028 (8)	0.0034 (8)
C5	0.0283 (12)	0.0221 (11)	0.0187 (11)	0.0083 (8)	−0.0055 (8)	−0.0035 (8)
C6	0.0217 (10)	0.0178 (10)	0.0238 (11)	0.0035 (8)	−0.0058 (9)	−0.0047 (8)
C7	0.0146 (9)	0.0158 (9)	0.0192 (9)	0.0025 (7)	−0.0044 (7)	0.0024 (7)
C8	0.0156 (9)	0.0163 (9)	0.0209 (10)	0.0009 (7)	−0.0049 (8)	0.0007 (7)
C9	0.0137 (9)	0.0179 (10)	0.0147 (9)	0.0006 (7)	0.0030 (7)	0.0015 (7)
C10	0.0158 (9)	0.0136 (9)	0.0148 (9)	−0.0017 (7)	0.0042 (7)	0.0015 (7)
C11	0.0141 (8)	0.0149 (9)	0.0123 (8)	−0.0039 (7)	0.0026 (7)	0.0009 (7)

Geometric parameters (Å, º)

S1—C11	1.6758 (19)	C1—C2	1.486 (2)
O1—C1	1.221 (2)	C2—C3	1.379 (3)
O2—C8	1.206 (2)	C2—C7	1.393 (3)
N1—C1	1.383 (2)	C3—C4	1.393 (3)
N1—C8	1.405 (2)	C3—H3	0.9500
N1—C9	1.447 (2)	C4—C5	1.391 (3)
N2—C10	1.369 (2)	C4—H4	0.9500
N2—C11	1.374 (2)	C5—C6	1.399 (3)
N2—N5	1.404 (2)	C5—H5	0.9500
N3—C11	1.339 (2)	C6—C7	1.378 (3)
N3—N4	1.384 (2)	C6—H6	0.9500
N3—H3N	0.84 (2)	C7—C8	1.485 (3)
N4—C10	1.297 (2)	C9—C10	1.492 (3)
N5—H5M	0.92 (2)	C9—H9A	0.9900
N5—H5N	0.83 (2)	C9—H9B	0.9900
C1—N1—C8	112.26 (15)	C4—C5—C6	120.62 (18)
C1—N1—C9	124.53 (16)	C4—C5—H5	119.7
C8—N1—C9	122.97 (16)	C6—C5—H5	119.7
C10—N2—C11	108.51 (15)	C7—C6—C5	117.51 (19)
C10—N2—N5	123.96 (16)	C7—C6—H6	121.2
C11—N2—N5	127.49 (15)	C5—C6—H6	121.2
C11—N3—N4	113.71 (16)	C6—C7—C2	121.57 (18)

C11—N3—H3N	128.9 (17)	C6—C7—C8	130.00 (18)
N4—N3—H3N	116.8 (16)	C2—C7—C8	108.41 (15)
C10—N4—N3	103.49 (15)	O2—C8—N1	124.66 (19)
N2—N5—H5M	107.6 (14)	O2—C8—C7	130.08 (18)
N2—N5—H5N	102.3 (14)	N1—C8—C7	105.26 (15)
H5M—N5—H5N	111 (2)	N1—C9—C10	112.97 (14)
O1—C1—N1	123.71 (17)	N1—C9—H9A	109.0
O1—C1—C2	130.07 (17)	C10—C9—H9A	109.0
N1—C1—C2	106.21 (15)	N1—C9—H9B	109.0
C3—C2—C7	121.38 (17)	C10—C9—H9B	109.0
C3—C2—C1	130.85 (18)	H9A—C9—H9B	107.8
C7—C2—C1	107.77 (15)	N4—C10—N2	111.40 (16)
C2—C3—C4	117.30 (18)	N4—C10—C9	123.90 (16)
C2—C3—H3	121.4	N2—C10—C9	124.69 (16)
C4—C3—H3	121.4	N3—C11—N2	102.87 (15)
C5—C4—C3	121.58 (18)	N3—C11—S1	129.02 (15)
C5—C4—H4	119.2	N2—C11—S1	128.09 (14)
C3—C4—H4	119.2		

C11—N3—N4—C10	−1.5 (2)	C1—N1—C8—C7	3.1 (2)
C8—N1—C1—O1	176.97 (17)	C9—N1—C8—C7	177.81 (15)
C9—N1—C1—O1	2.3 (3)	C6—C7—C8—O2	−3.0 (3)
C8—N1—C1—C2	−2.7 (2)	C2—C7—C8—O2	178.56 (19)
C9—N1—C1—C2	−177.36 (16)	C6—C7—C8—N1	176.21 (18)
O1—C1—C2—C3	1.0 (3)	C2—C7—C8—N1	−2.19 (19)
N1—C1—C2—C3	−179.35 (18)	C1—N1—C9—C10	54.3 (2)
O1—C1—C2—C7	−178.46 (18)	C8—N1—C9—C10	−119.80 (18)
N1—C1—C2—C7	1.21 (19)	N3—N4—C10—N2	1.3 (2)
C7—C2—C3—C4	−1.5 (3)	N3—N4—C10—C9	−179.32 (16)
C1—C2—C3—C4	179.12 (19)	C11—N2—C10—N4	−0.7 (2)
C2—C3—C4—C5	−0.5 (3)	N5—N2—C10—N4	−178.54 (16)
C3—C4—C5—C6	1.6 (3)	C11—N2—C10—C9	179.92 (16)
C4—C5—C6—C7	−0.6 (3)	N5—N2—C10—C9	2.0 (3)
C5—C6—C7—C2	−1.4 (3)	N1—C9—C10—N4	−130.71 (18)
C5—C6—C7—C8	−179.66 (18)	N1—C9—C10—N2	48.6 (2)
C3—C2—C7—C6	2.6 (3)	N4—N3—C11—N2	1.11 (19)
C1—C2—C7—C6	−177.94 (17)	N4—N3—C11—S1	−177.21 (14)
C3—C2—C7—C8	−178.88 (17)	C10—N2—C11—N3	−0.28 (19)
C1—C2—C7—C8	0.62 (19)	N5—N2—C11—N3	177.50 (17)
C1—N1—C8—O2	−177.62 (17)	C10—N2—C11—S1	178.06 (14)
C9—N1—C8—O2	−2.9 (3)	N5—N2—C11—S1	−4.2 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5*M*···O2^{i}	0.92 (2)	2.29 (2)	3.151 (2)	155.6 (19)

N5—H5*N*···S1^{ii}	0.83 (2)	2.60 (2)	3.430 (2)	177.4 (18)
N3—H3*N*···O1^{iii}	0.84 (2)	1.98 (2)	2.811 (2)	169 (2)

Symmetry codes: (i) $x-1, y, z$; (ii) $x+1/2, -y+3/2, z$; (iii) $-x, -y+1, z-1/2$.