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Crystal structure of cyclosulfamuron

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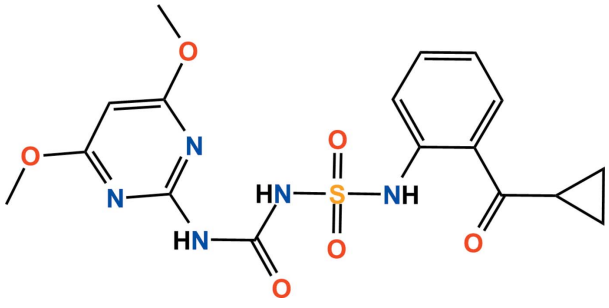
The title compound (systematic name: 1-{[2-(cyclopropylcarbonyl)anilino]sulfonyl}-3-(4,6-dimethoxypyrimidin-2-yl)urea), $C_{17}H_{19}N_5O_6S$, is a pyrimidinylsulfonylurea herbicide. The dihedral angles between the mean planes of the central benzene ring and the cyclopropyl and pyrimidinyl rings are 75.32 (9) and 88.79 (4)°, respectively. The C atoms of the methoxy groups lie almost in the plane of the pyrimidine ring [deviations = 0.043 (2) and 0.028 (2) Å] and intramolecular N—H···N, N—H···O and C—H···O hydrogen bonds all close *S*(6) rings. In the crystal, N—H···O and C—H···O hydrogen bonds and weak π–π interactions [centroid–centroid distances = 3.6175 (9) and 3.7068 (9) Å] link adjacent molecules, forming a three-dimensional network.

Keywords: crystal structure; hydrogen bonding; π–π interactions.

CCDC reference: 1415211

1. Related literature

For information on the herbicidal properties of the title compound, see: Sarıgül & İnam (2009). For a related crystal structure, see: Xia *et al.* (2008).



2. Experimental

2.1. Crystal data

$C_{17}H_{19}N_5O_6S$
M_r = 421.43
Monoclinic, $P2_1/n$
a = 12.7019 (4) Å
b = 9.6216 (3) Å
c = 15.6213 (5) Å
β = 93.6194 (12)°
V = 1905.31 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 173 K
0.32 × 0.27 × 0.23 mm

2.2. Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2013)
T_{min} = 0.934, T_{max} = 0.952
17544 measured reflections
4365 independent reflections
3688 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.113
S = 1.05
4365 reflections
264 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*···O1	0.88	1.86	2.5736 (18)	137
N2—H2*N*···N4	0.88	1.92	2.6158 (18)	135
C9—H9···O3	0.95	2.45	3.088 (2)	124
N3—H3*N*···O2^{i}	0.88	2.08	2.9391 (17)	165
C2—H2*B*···O2^{ii}	0.99	2.51	3.483 (2)	169
C3—H3···O4^{iii}	1.00	2.51	3.286 (2)	135
C8—H8···O3^{iv}	0.95	2.50	3.307 (2)	142

Symmetry codes: (i) $-x+\frac{5}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+2, -y+1, -z$; (iii) $-x+2, -y, -z$; (iv) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2013); cell refinement: *SAINT* (Bruker, 2013); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2015); molecular graphics: *DIAMOND* (Brandenburg, 2010); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7470).

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supporting information

Acta Cryst. (2015). E**71**, o631–o632 [https://doi.org/10.1107/S2056989015014115]

Crystal structure of cyclosulfamuron

Gihaeng Kang, Jineun Kim, Eunjin Kwon and Tae Ho Kim

S1. Comment

Cyclosulfamuron [systematic name: 1-[2-(cyclopropylcarbonyl)anilinosulfonyl]-3-(4,6-dimethoxypyrimidin-2-yl)urea] is a pyrimidinylsulfonylurea herbicide and has been widely used to control weeds because of their low toxicity to mammals and their high herbicidal activity (Sarıgül & Inam, 2009). However, until now its crystal structure has not been reported. In the title compound (Fig. 1), the dihedral angles between the mean planes of the central phenyl ring and the cyclopropyl and pyrimidinyl rings are 75.32 (9) and 88.79 (4)°, respectively. All bond lengths and bond angles are normal and comparable to those observed in a similar crystal structure (Xia *et al.*, 2008).

In the crystal structure (Fig. 2), N—H···O and C—H···O hydrogen bonds are observed (Table 1). In addition, weak intermolecular *Cg*1···*Cg*1^{v} and *Cg*1···*Cg*2^{vi} (*Cg*1 and *Cg*2 are the centroids of the N4—C12—N5—C15—C14—C13 and C5–C10 rings, respectively) interactions are present [for symmetry codes: (v), -*x* + 2, -*y*, -*z* + 1, (vi), *x* + 1/2, -*y* + 1/2, *z* + 1/2]. A three-dimensional network is formed by the hydrogen bonds and π–π interactions.

S2. Experimental

The title compound was purchased from the Dr. Ehrenstorfer GmbH Company. Slow evaporation of a solution in CH_2Cl_2 gave single crystals suitable for X-ray analysis.

S3. Refinement

All H-atoms were positioned geometrically and refined using a riding model with d(N—H) = 0.88 Å, U_{iso} = 1.2U_{eq}(C) for N—H group, d(C—H) = 1.00 Å, U_{iso} = 1.2U_{eq}(C) for Csp^3—H. d(C—H) = 0.98 Å, U_{iso} = 1.5U_{eq}(C) for methyl group, d(C—H) = 0.99 Å, U_{iso} = 1.2U_{eq}(C) for CH_2 group, d(C—H) = 0.95 Å, U_{iso} = 1.2U_{eq}(C) for aromatic C—H.

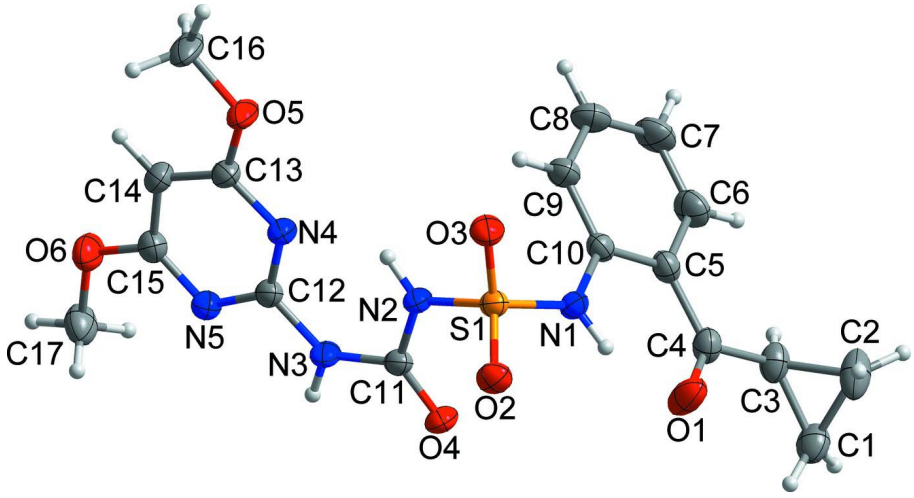

Figure 1

The asymmetric unit of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radius.

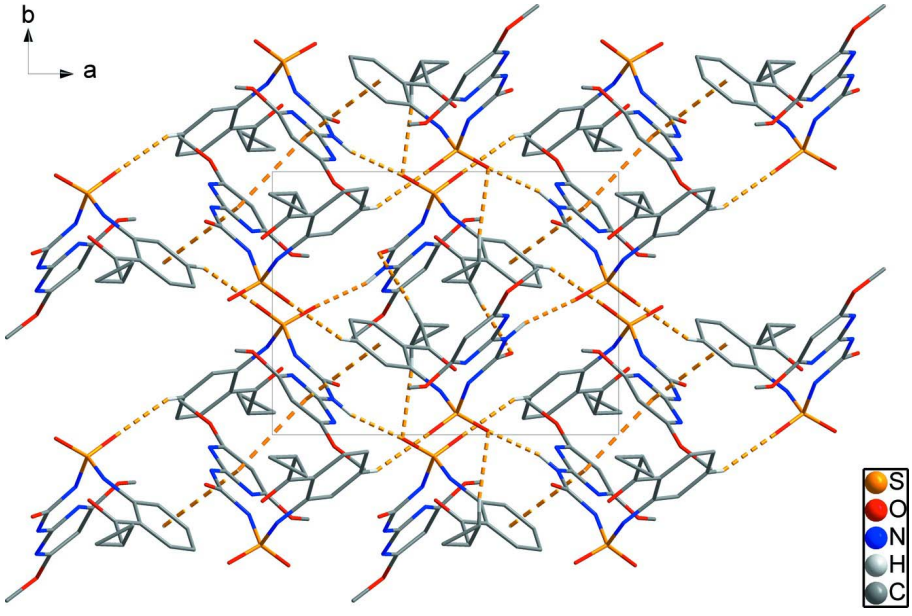

Figure 2

Crystal packing viewed along the *c* axis. The intermolecular interactions are shown as dashed lines.

1-{[2-(Cyclopropylcarbonyl)anilino]sulfonyl}-3-(4,6-dimethoxypyrimidin-2-yl)urea

Crystal data

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$c = 15.6213\ (5)$ Å
$\beta = 93.6194\ (12)°$
$V = 1905.31\ (10)$ Å^3
$Z = 4$
$F(000) = 880$
$D_x = 1.469$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6977 reflections
$\theta = 2.6–27.4°$

μ = 0.22 mm^{-1}
T = 173 K

Block, colourless
0.32 × 0.27 × 0.23 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2013)
T_{min} = 0.934, T_{max} = 0.952
17544 measured reflections

4365 independent reflections
3688 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 27.5°, θ_{min} = 2.0°
h = −16→15
k = −12→12
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.113
S = 1.05
4365 reflections
264 parameters
0 restraints

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0579P)^2 + 0.7248P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
S1	1.03274 (3)	0.41778 (4)	0.19915 (2)	0.02564 (12)
O1	1.02757 (11)	0.25129 (16)	−0.03440 (8)	0.0524 (4)
O2	1.12410 (9)	0.48608 (12)	0.17159 (7)	0.0340 (3)
O3	0.95254 (9)	0.49585 (12)	0.23699 (7)	0.0343 (3)
O4	1.19071 (9)	0.18921 (12)	0.19997 (7)	0.0335 (3)
O5	0.94327 (9)	0.31556 (13)	0.52112 (7)	0.0386 (3)
O6	1.17908 (10)	−0.04334 (14)	0.61128 (7)	0.0429 (3)
N1	0.98567 (10)	0.33405 (14)	0.11638 (8)	0.0290 (3)
H1N	1.0187	0.3456	0.0690	0.035*
N2	1.06665 (10)	0.30293 (14)	0.27345 (8)	0.0281 (3)
H2N	1.0317	0.3014	0.3203	0.034*
N3	1.17533 (10)	0.13526 (15)	0.33969 (8)	0.0303 (3)
H3N	1.2279	0.0767	0.3351	0.036*
N4	1.05707 (10)	0.22678 (14)	0.43352 (8)	0.0284 (3)
N5	1.17993 (10)	0.04736 (14)	0.47520 (8)	0.0302 (3)
C1	1.00581 (16)	0.0853 (2)	−0.18258 (11)	0.0418 (4)
H1A	1.0695	0.1442	−0.1740	0.050*
H1B	1.0162	−0.0019	−0.2147	0.050*
C2	0.90252 (18)	0.1560 (2)	−0.19567 (11)	0.0492 (5)
H2A	0.8486	0.1127	−0.2357	0.059*

H2B	0.9019	0.2589	−0.1950	0.059*
C3	0.93094 (14)	0.08205 (17)	−0.11251 (10)	0.0354 (4)
H3	0.8943	−0.0082	−0.1031	0.042*
C4	0.95231 (14)	0.17112 (17)	−0.03618 (10)	0.0334 (4)
C5	0.88087 (12)	0.16383 (17)	0.03524 (10)	0.0301 (3)
C6	0.79319 (14)	0.0755 (2)	0.02989 (12)	0.0415 (4)
H6	0.7797	0.0215	−0.0206	0.050*
C7	0.72575 (15)	0.0639 (2)	0.09523 (13)	0.0462 (5)
H7	0.6672	0.0023	0.0901	0.055*
C8	0.74454 (14)	0.1432 (2)	0.16818 (12)	0.0432 (4)
H8	0.6987	0.1354	0.2137	0.052*
C9	0.82919 (13)	0.23370 (19)	0.17609 (10)	0.0347 (4)
H9	0.8403	0.2886	0.2264	0.042*
C10	0.89805 (12)	0.24451 (16)	0.11062 (9)	0.0267 (3)
C11	1.14737 (12)	0.20858 (16)	0.26595 (9)	0.0267 (3)
C12	1.13446 (12)	0.13831 (16)	0.42007 (9)	0.0272 (3)
C13	1.01967 (12)	0.22237 (17)	0.51212 (9)	0.0294 (3)
C14	1.05796 (13)	0.13144 (18)	0.57482 (9)	0.0325 (4)
H14	1.0303	0.1274	0.6299	0.039*
C15	1.13996 (13)	0.04587 (18)	0.55188 (10)	0.0314 (3)
C16	0.89737 (16)	0.3201 (2)	0.60284 (11)	0.0514 (5)
H16A	0.8605	0.2326	0.6124	0.077*
H16B	0.8472	0.3974	0.6035	0.077*
H16C	0.9531	0.3336	0.6484	0.077*
C17	1.26553 (16)	−0.1300 (2)	0.58797 (12)	0.0463 (5)
H17A	1.2435	−0.1851	0.5372	0.069*
H17B	1.2862	−0.1925	0.6357	0.069*
H17C	1.3256	−0.0714	0.5752	0.069*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0234 (2)	0.0291 (2)	0.02454 (19)	−0.00228 (14)	0.00254 (14)	−0.00382 (13)
O1	0.0535 (9)	0.0729 (10)	0.0323 (6)	−0.0295 (7)	0.0133 (6)	−0.0169 (6)
O2	0.0313 (6)	0.0348 (6)	0.0362 (6)	−0.0109 (5)	0.0052 (5)	−0.0047 (5)
O3	0.0321 (6)	0.0368 (6)	0.0343 (6)	0.0076 (5)	0.0039 (5)	−0.0045 (5)
O4	0.0305 (6)	0.0445 (7)	0.0263 (5)	0.0045 (5)	0.0096 (4)	−0.0049 (5)
O5	0.0368 (7)	0.0544 (8)	0.0255 (6)	0.0162 (6)	0.0090 (5)	−0.0010 (5)
O6	0.0459 (8)	0.0518 (8)	0.0309 (6)	0.0133 (6)	0.0007 (5)	0.0070 (5)
N1	0.0263 (7)	0.0387 (7)	0.0222 (6)	−0.0083 (6)	0.0039 (5)	−0.0029 (5)
N2	0.0243 (7)	0.0385 (7)	0.0221 (6)	0.0048 (5)	0.0055 (5)	−0.0010 (5)
N3	0.0256 (7)	0.0394 (7)	0.0263 (6)	0.0096 (6)	0.0059 (5)	−0.0015 (5)
N4	0.0253 (7)	0.0370 (7)	0.0232 (6)	0.0037 (5)	0.0039 (5)	−0.0023 (5)
N5	0.0263 (7)	0.0368 (7)	0.0274 (6)	0.0026 (6)	0.0016 (5)	−0.0017 (5)
C1	0.0512 (11)	0.0429 (10)	0.0312 (8)	0.0058 (8)	0.0010 (8)	−0.0081 (7)
C2	0.0760 (15)	0.0388 (10)	0.0310 (9)	0.0193 (10)	−0.0112 (9)	−0.0048 (7)
C3	0.0467 (10)	0.0305 (8)	0.0283 (8)	0.0018 (7)	−0.0033 (7)	−0.0030 (6)
C4	0.0368 (9)	0.0366 (9)	0.0262 (7)	−0.0024 (7)	−0.0031 (6)	−0.0015 (6)

C5	0.0270 (8)	0.0333 (8)	0.0292 (7)	−0.0029 (6)	−0.0049 (6)	0.0009 (6)
C6	0.0348 (10)	0.0436 (10)	0.0451 (10)	−0.0099 (8)	−0.0048 (8)	−0.0083 (8)
C7	0.0301 (9)	0.0511 (11)	0.0571 (11)	−0.0163 (8)	−0.0002 (8)	−0.0050 (9)
C8	0.0282 (9)	0.0552 (11)	0.0471 (10)	−0.0093 (8)	0.0086 (7)	0.0018 (9)
C9	0.0255 (8)	0.0450 (10)	0.0338 (8)	−0.0062 (7)	0.0027 (6)	−0.0025 (7)
C10	0.0220 (7)	0.0304 (8)	0.0272 (7)	−0.0022 (6)	−0.0019 (6)	0.0015 (6)
C11	0.0209 (7)	0.0342 (8)	0.0252 (7)	−0.0015 (6)	0.0030 (5)	−0.0046 (6)
C12	0.0234 (7)	0.0346 (8)	0.0238 (7)	−0.0015 (6)	0.0017 (6)	−0.0037 (6)
C13	0.0260 (8)	0.0379 (8)	0.0244 (7)	0.0015 (6)	0.0033 (6)	−0.0057 (6)
C14	0.0328 (9)	0.0429 (9)	0.0220 (7)	0.0020 (7)	0.0036 (6)	−0.0029 (6)
C15	0.0287 (8)	0.0383 (9)	0.0270 (7)	−0.0005 (7)	−0.0013 (6)	−0.0006 (6)
C16	0.0513 (12)	0.0780 (15)	0.0262 (8)	0.0277 (11)	0.0122 (8)	−0.0043 (9)
C17	0.0476 (11)	0.0523 (11)	0.0379 (9)	0.0167 (9)	−0.0058 (8)	0.0016 (8)

Geometric parameters (Å, º)

S1—O2	1.4237 (11)	C2—C3	1.505 (2)
S1—O3	1.4238 (11)	C2—H2A	0.9900
S1—N1	1.6065 (12)	C2—H2B	0.9900
S1—N2	1.6402 (13)	C3—C4	1.480 (2)
O1—C4	1.227 (2)	C3—H3	1.0000
O4—C11	1.2132 (17)	C4—C5	1.484 (2)
O5—C13	1.3351 (19)	C5—C6	1.399 (2)
O5—C16	1.4372 (19)	C5—C10	1.416 (2)
O6—C15	1.3366 (19)	C6—C7	1.378 (3)
O6—C17	1.444 (2)	C6—H6	0.9500
N1—C10	1.4058 (19)	C7—C8	1.379 (3)
N1—H1N	0.8800	C7—H7	0.9500
N2—C11	1.3799 (19)	C8—C9	1.383 (2)
N2—H2N	0.8800	C8—H8	0.9500
N3—C11	1.378 (2)	C9—C10	1.391 (2)
N3—C12	1.3890 (18)	C9—H9	0.9500
N3—H3N	0.8800	C13—C14	1.379 (2)
N4—C12	1.327 (2)	C14—C15	1.392 (2)
N4—C13	1.3449 (19)	C14—H14	0.9500
N5—C15	1.3303 (19)	C16—H16A	0.9800
N5—C12	1.333 (2)	C16—H16B	0.9800
C1—C2	1.480 (3)	C16—H16C	0.9800
C1—C3	1.495 (2)	C17—H17A	0.9800
C1—H1A	0.9900	C17—H17B	0.9800
C1—H1B	0.9900	C17—H17C	0.9800
O2—S1—O3	120.02 (7)	C7—C6—C5	122.31 (17)
O2—S1—N1	104.90 (7)	C7—C6—H6	118.8
O3—S1—N1	111.04 (7)	C5—C6—H6	118.8
O2—S1—N2	110.02 (7)	C6—C7—C8	118.96 (17)
O3—S1—N2	102.97 (7)	C6—C7—H7	120.5
N1—S1—N2	107.42 (7)	C8—C7—H7	120.5

C13—O5—C16	116.90 (13)	C7—C8—C9	120.99 (17)
C15—O6—C17	116.82 (13)	C7—C8—H8	119.5
C10—N1—S1	127.72 (10)	C9—C8—H8	119.5
C10—N1—H1N	116.1	C8—C9—C10	120.18 (16)
S1—N1—H1N	116.1	C8—C9—H9	119.9
C11—N2—S1	123.13 (10)	C10—C9—H9	119.9
C11—N2—H2N	118.4	C9—C10—N1	122.06 (14)
S1—N2—H2N	118.4	C9—C10—C5	119.97 (14)
C11—N3—C12	130.81 (13)	N1—C10—C5	117.98 (13)
C11—N3—H3N	114.6	O4—C11—N3	121.65 (14)
C12—N3—H3N	114.6	O4—C11—N2	123.54 (14)
C12—N4—C13	115.60 (13)	N3—C11—N2	114.81 (12)
C15—N5—C12	114.47 (13)	N4—C12—N5	127.86 (14)
C2—C1—C3	60.76 (12)	N4—C12—N3	118.65 (14)
C2—C1—H1A	117.7	N5—C12—N3	113.49 (13)
C3—C1—H1A	117.7	O5—C13—N4	112.08 (13)
C2—C1—H1B	117.7	O5—C13—C14	125.27 (14)
C3—C1—H1B	117.7	N4—C13—C14	122.65 (14)
H1A—C1—H1B	114.8	C13—C14—C15	115.36 (14)
C1—C2—C3	60.10 (12)	C13—C14—H14	122.3
C1—C2—H2A	117.8	C15—C14—H14	122.3
C3—C2—H2A	117.8	N5—C15—O6	119.06 (15)
C1—C2—H2B	117.8	N5—C15—C14	124.04 (15)
C3—C2—H2B	117.8	O6—C15—C14	116.89 (14)
H2A—C2—H2B	114.9	O5—C16—H16A	109.5
C4—C3—C1	119.02 (16)	O5—C16—H16B	109.5
C4—C3—C2	116.34 (14)	H16A—C16—H16B	109.5
C1—C3—C2	59.14 (12)	O5—C16—H16C	109.5
C4—C3—H3	116.6	H16A—C16—H16C	109.5
C1—C3—H3	116.6	H16B—C16—H16C	109.5
C2—C3—H3	116.6	O6—C17—H17A	109.5
O1—C4—C3	119.04 (15)	O6—C17—H17B	109.5
O1—C4—C5	121.68 (14)	H17A—C17—H17B	109.5
C3—C4—C5	119.26 (15)	O6—C17—H17C	109.5
C6—C5—C10	117.59 (15)	H17A—C17—H17C	109.5
C6—C5—C4	120.40 (15)	H17B—C17—H17C	109.5
C10—C5—C4	122.01 (14)		

O2—S1—N1—C10	176.89 (13)	C4—C5—C10—C9	−179.69 (15)
O3—S1—N1—C10	−52.05 (15)	C6—C5—C10—N1	−179.72 (15)
N2—S1—N1—C10	59.84 (15)	C4—C5—C10—N1	0.3 (2)
O2—S1—N2—C11	−47.34 (14)	C12—N3—C11—O4	−177.90 (15)
O3—S1—N2—C11	−176.41 (12)	C12—N3—C11—N2	1.5 (2)
N1—S1—N2—C11	66.31 (13)	S1—N2—C11—O4	−10.3 (2)
C2—C1—C3—C4	−105.05 (18)	S1—N2—C11—N3	170.31 (11)
C1—C2—C3—C4	109.56 (18)	C13—N4—C12—N5	−0.8 (2)
C1—C3—C4—O1	4.1 (2)	C13—N4—C12—N3	178.68 (14)
C2—C3—C4—O1	−63.6 (2)	C15—N5—C12—N4	1.3 (2)

C1—C3—C4—C5	−177.36 (15)	C15—N5—C12—N3	−178.23 (14)
C2—C3—C4—C5	114.96 (19)	C11—N3—C12—N4	−2.0 (2)
O1—C4—C5—C6	177.40 (17)	C11—N3—C12—N5	177.54 (15)
C3—C4—C5—C6	−1.1 (2)	C16—O5—C13—N4	−179.99 (16)
O1—C4—C5—C10	−2.6 (3)	C16—O5—C13—C14	−0.3 (2)
C3—C4—C5—C10	178.88 (14)	C12—N4—C13—O5	179.06 (13)
C10—C5—C6—C7	−1.0 (3)	C12—N4—C13—C14	−0.6 (2)
C4—C5—C6—C7	179.00 (18)	O5—C13—C14—C15	−178.31 (15)
C5—C6—C7—C8	0.7 (3)	N4—C13—C14—C15	1.3 (2)
C6—C7—C8—C9	0.4 (3)	C12—N5—C15—O6	178.96 (14)
C7—C8—C9—C10	−1.0 (3)	C12—N5—C15—C14	−0.4 (2)
C8—C9—C10—N1	−179.31 (16)	C17—O6—C15—N5	1.8 (2)
C8—C9—C10—C5	0.7 (3)	C17—O6—C15—C14	−178.78 (15)
S1—N1—C10—C9	10.3 (2)	C13—C14—C15—N5	−0.8 (2)
S1—N1—C10—C5	−169.74 (12)	C13—C14—C15—O6	179.85 (15)
C6—C5—C10—C9	0.3 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*···O1	0.88	1.86	2.5736 (18)	137
N2—H2*N*···N4	0.88	1.92	2.6158 (18)	135
C9—H9···O3	0.95	2.45	3.088 (2)	124
N3—H3*N*···O2^{i}	0.88	2.08	2.9391 (17)	165
C2—H2*B*···O2^{ii}	0.99	2.51	3.483 (2)	169
C3—H3···O4^{iii}	1.00	2.51	3.286 (2)	135
C8—H8···O3^{iv}	0.95	2.50	3.307 (2)	142

Symmetry codes: (i) −*x*+5/2, *y*−1/2, −*z*+1/2; (ii) −*x*+2, −*y*+1, −*z*; (iii) −*x*+2, −*y*, −*z*; (iv) −*x*+3/2, *y*−1/2, −*z*+1/2.