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N-(4-Hydroxyphenyl)-2-(1,1,3-trioxo-2,3-dihydro-1,2-benzothiazol-2-yl)-acetamide

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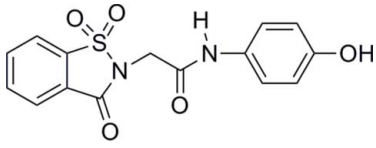
Key indicators: single-crystal X-ray study; T = 230 K; mean σ(C–C) = 0.004 Å; R factor = 0.039; wR factor = 0.084; data-to-parameter ratio = 13.9.

In the title compound, $C_{15}H_{12}N_2O_5S$, the benzisothiazole group is approximately planar (r.m.s. deviation excluding H atoms and the two O atoms bonded to S = 0.023 Å). The dihedral angle between the benzisothiazole ring and the terminal phenol ring is 84.9 (1)°. In the crystal, molecules are joined by N—H···O and O—H···O hydrogen bonds, and π-stacking interactions are observed between alternating phenol and benzisothiazole rings [centroid–centroid distances = 3.929 (3) and 3.943 (3) Å].

Related literature

For background literature related to analgesics, see: Slattery *et al.* (1996); McGoldrick & Bailie (1997); Watkins *et al.* (2006). For the synthesis and biological activity of the title compound, see: Vaccarino *et al.* (2007); González-Martin *et al.* (1998); Bazan & Alvarez-Builla (1996*a*,*b*). For related structures, see: Arshad *et al.* (2009*a*,*b*,*c*); Siddiqui *et al.* (2008*a*,*b*; 2007).



Experimental

Crystal data

$C_{15}H_{12}N_2O_5S$
M_r = 332.33
Orthorhombic, $Pna2_1$
a = 16.3588 (10) Å
b = 9.6451 (6) Å
c = 9.9603 (6) Å
V = 1571.56 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 230 K
0.60 × 0.20 × 0.20 mm

Data collection

Bruker SMART 1K CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.832, T_{max} = 0.954
19429 measured reflections
3580 independent reflections
3283 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.084
S = 1.07
3580 reflections
257 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}
Absolute structure: Flack (1983), 1681 Friedel pairs
Flack parameter: 0.02 (8)

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

D—H···A	D—H	H···A	D···A	D—H···A
N10—H10···O14^{i}	0.87 (3)	2.23 (3)	3.078 (3)	165 (3)
O14—H14···O9^{ii}	0.82 (3)	1.91 (3)	2.725 (2)	173 (3)

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; 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*.

Helpful discussions with Professor M. L. Trudell, University of New Orleans, are gratefully acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2377).

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supporting information

Acta Cryst. (2009). E**65**, o1667 [doi:10.1107/S1600536809023022]

N-(4-Hydroxyphenyl)-2-(1,1,3-trioxo-2,3-dihydro-1,2-benzothiazol-2-yl)acetamide

Abha Verma and Edwin D. Stevens

S1. Comment

Analgesics currently in use have high incidence of adverse reactions and can cause potentially lethal effects like hepatotoxicity and nephrotoxicity (Slattery *et al.*, 1996; McGoldrick & Bailie, 1997; Watkins *et al.*, 2006). A series of compounds bearing the acetaminophen (Tylenol) fragment linked to different lipophilic heterocyclic moieties were synthesized with a view to modulate its pharmacokinetic profile (Bazan & Alvarez-Builla, 1996*a*,*b*6; Vaccarino *et al.*, 2007). Of these new derivatives, the title compound (commonly called SCP-1) has a similar profile to that of acetaminophen but with shorter elimination half-life and clearance.

S2. Experimental

The title compound was synthesized following the procedure described by Vaccarino *et al.* (2007) and colourless needles suitable for X-ray analysis were obtained by recrystallization from an ethanol-water (8:1) mixture.

S3. Refinement

All H atoms were located in a difference density map and their positional parameters and U_{iso} included in the full-matrix least-squares refinement. Observed C—H bond lengths are in the range 0.91 (3)–0.97 (3) Å.

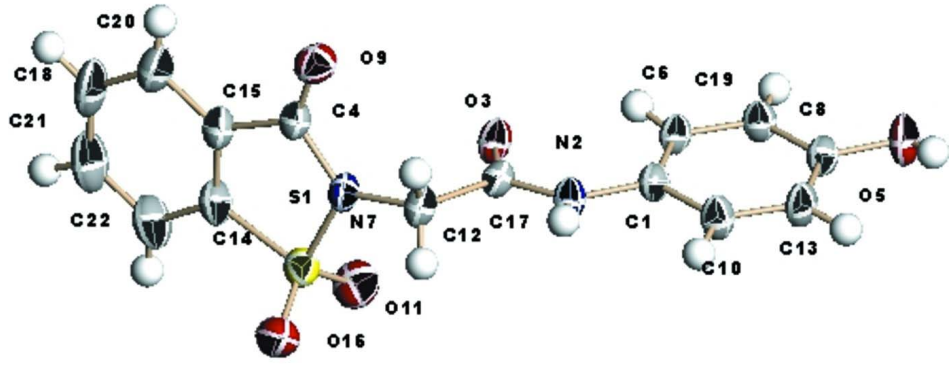

Figure 1

The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

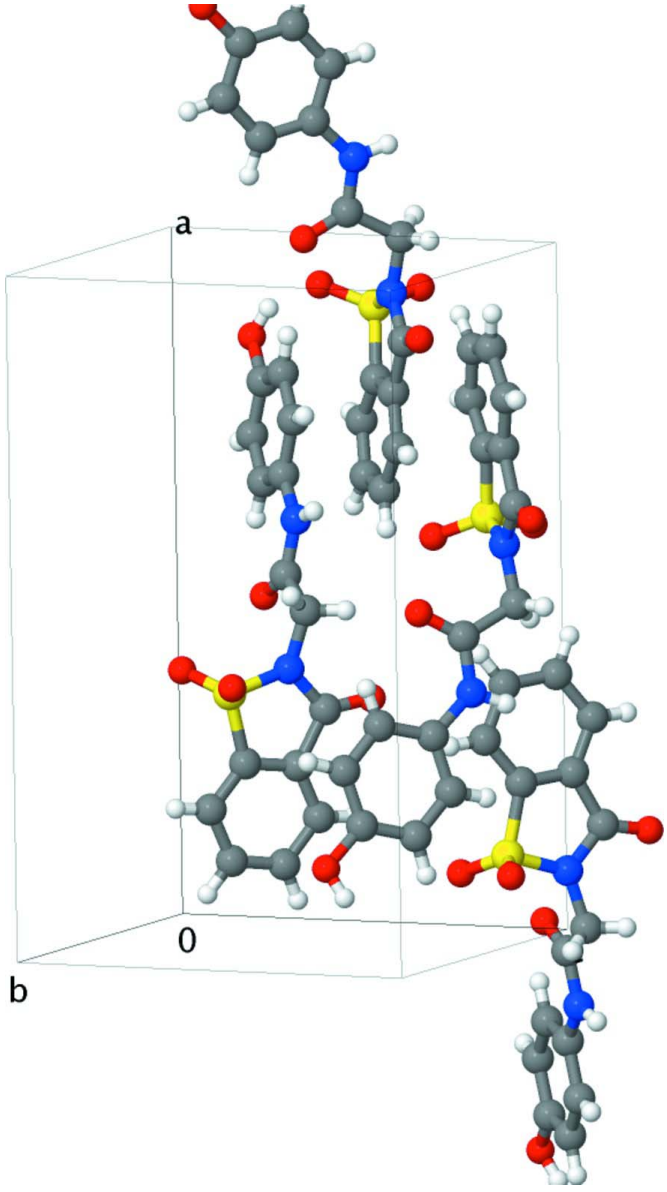

Figure 2

Perspective view of the contents of the unit cell showing the parallel stacking of the aromatic rings in layers perpendicular to the a axis.

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Crystal data

$C_{15}H_{12}N_2O_5S$
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Orthorhombic, $Pna2_1$
Hall symbol: P 2c -2n
$a = 16.3588\ (10)$ Å
$b = 9.6451\ (6)$ Å
$c = 9.9603\ (6)$ Å
$V = 1571.56\ (17)$ Å^3
$Z = 4$
$F(000) = 688$
$D_x = 1.405$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 17706 reflections
$\theta = 2.5–30.5°$
$\mu = 0.23$ mm^{-1}
$T = 230$ K
Needle, colourless
0.60 × 0.20 × 0.20 mm

Data collection

Bruker SMART 1K CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.832, T_{max} = 0.954
19429 measured reflections
3580 independent reflections
3283 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 27.5°, θ_{min} = 2.5°
h = −21→21
k = −12→12
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.084
S = 1.07
3580 reflections
257 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
$w = 1/[\sigma^2(F_o^2) + (0.0183P)^2 + 1.0724P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0063 (8)
Absolute structure: Flack (1983), 1681 Friedel pairs
Absolute structure parameter: 0.02 (8)

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	0.11997 (4)	0.20573 (6)	0.93772 (6)	0.03830 (15)
O1	0.10058 (12)	0.3352 (2)	1.0007 (2)	0.0534 (5)
N2	0.09100 (11)	0.0757 (2)	1.0375 (2)	0.0339 (4)
O2	0.08966 (13)	0.1841 (2)	0.80485 (18)	0.0554 (5)
C3	0.15368 (14)	0.0026 (2)	1.0986 (2)	0.0320 (5)
O3	0.14167 (11)	−0.0882 (2)	1.17895 (19)	0.0451 (4)
C4	0.31014 (15)	0.0065 (3)	1.0784 (3)	0.0467 (6)
H4	0.3137 (16)	−0.067 (3)	1.135 (3)	0.034 (7)*
C4A	0.23289 (14)	0.0552 (3)	1.0467 (2)	0.0353 (5)
C5	0.37621 (17)	0.0677 (4)	1.0128 (4)	0.0608 (9)
H5	0.430 (2)	0.035 (4)	1.032 (4)	0.081 (11)*
C6	0.36573 (17)	0.1721 (4)	0.9215 (4)	0.0640 (9)
H6	0.4123 (19)	0.209 (3)	0.873 (4)	0.065 (9)*

C7A	0.22384 (13)	0.1609 (3)	0.9562 (3)	0.0398 (5)
C7	0.2887 (2)	0.2225 (3)	0.8913 (3)	0.0561 (8)
H7	0.283 (2)	0.295 (3)	0.830 (3)	0.058 (9)*
C8	0.00639 (14)	0.0545 (3)	1.0733 (2)	0.0346 (5)
H8B	−0.0203 (16)	0.141 (3)	1.072 (3)	0.038 (7)*
H8A	0.0067 (16)	0.018 (3)	1.162 (3)	0.035 (7)*
C9	−0.03588 (12)	−0.0469 (2)	0.9791 (2)	0.0298 (4)
O9	0.00080 (9)	−0.11209 (18)	0.89225 (16)	0.0379 (4)
N10	−0.11625 (11)	−0.0573 (2)	1.0033 (2)	0.0331 (4)
H10	−0.1339 (17)	−0.008 (3)	1.070 (3)	0.045 (8)*
C11	−0.17479 (12)	−0.1418 (2)	0.9368 (2)	0.0295 (4)
C12	−0.25630 (14)	−0.1228 (3)	0.9725 (3)	0.0391 (6)
H12	−0.2690 (17)	−0.049 (3)	1.033 (3)	0.047 (8)*
C13	−0.31719 (13)	−0.2010 (3)	0.9129 (3)	0.0407 (6)
H13	−0.3736 (19)	−0.187 (3)	0.933 (4)	0.066 (9)*
C14	−0.29711 (13)	−0.2994 (2)	0.8175 (2)	0.0320 (5)
O14	−0.35473 (10)	−0.3808 (2)	0.75619 (19)	0.0442 (5)
H14	−0.397 (2)	−0.378 (3)	0.802 (4)	0.060 (10)*
C15	−0.21627 (14)	−0.3179 (3)	0.7811 (2)	0.0341 (5)
H15	−0.2007 (16)	−0.386 (3)	0.716 (3)	0.040 (7)*
C16	−0.15511 (13)	−0.2396 (3)	0.8404 (2)	0.0320 (5)
H16	−0.1000 (17)	−0.255 (3)	0.814 (3)	0.041 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0371 (3)	0.0407 (3)	0.0371 (3)	−0.0060 (2)	−0.0064 (3)	0.0063 (3)
O1	0.0547 (11)	0.0422 (10)	0.0633 (12)	0.0011 (9)	−0.0100 (10)	0.0011 (9)
N2	0.0253 (9)	0.0422 (11)	0.0343 (10)	−0.0052 (8)	−0.0035 (7)	0.0048 (9)
O2	0.0640 (12)	0.0651 (13)	0.0371 (10)	−0.0036 (11)	−0.0141 (9)	0.0105 (9)
C3	0.0288 (11)	0.0366 (12)	0.0306 (11)	−0.0023 (9)	−0.0040 (9)	−0.0026 (10)
O3	0.0430 (10)	0.0481 (11)	0.0443 (10)	0.0011 (8)	−0.0010 (8)	0.0133 (9)
C4	0.0312 (12)	0.0594 (17)	0.0496 (15)	0.0012 (12)	−0.0040 (11)	−0.0117 (14)
C4A	0.0278 (11)	0.0438 (13)	0.0343 (11)	−0.0037 (10)	−0.0027 (10)	−0.0065 (10)
C5	0.0260 (13)	0.081 (2)	0.075 (2)	−0.0045 (14)	−0.0007 (13)	−0.0239 (19)
C6	0.0398 (14)	0.081 (2)	0.072 (2)	−0.0244 (15)	0.0125 (16)	−0.009 (2)
C7A	0.0312 (11)	0.0480 (13)	0.0401 (14)	−0.0085 (10)	0.0011 (10)	−0.0019 (11)
C7	0.0491 (16)	0.065 (2)	0.0547 (18)	−0.0222 (15)	0.0078 (13)	0.0049 (15)
C8	0.0256 (10)	0.0460 (14)	0.0323 (12)	−0.0015 (10)	−0.0004 (9)	−0.0030 (11)
C9	0.0246 (9)	0.0372 (11)	0.0275 (10)	−0.0002 (9)	−0.0012 (8)	0.0020 (9)
O9	0.0238 (7)	0.0520 (10)	0.0379 (9)	−0.0013 (7)	0.0043 (6)	−0.0089 (8)
N10	0.0249 (9)	0.0425 (11)	0.0319 (10)	−0.0037 (8)	0.0045 (8)	−0.0087 (9)
C11	0.0240 (8)	0.0352 (10)	0.0293 (9)	−0.0040 (8)	0.0016 (9)	−0.0002 (10)
C12	0.0276 (10)	0.0465 (14)	0.0432 (14)	−0.0007 (10)	0.0078 (10)	−0.0145 (11)
C13	0.0219 (10)	0.0511 (13)	0.0492 (16)	−0.0017 (10)	0.0059 (10)	−0.0093 (12)
C14	0.0254 (10)	0.0402 (12)	0.0304 (11)	−0.0067 (9)	0.0012 (9)	0.0024 (9)
O14	0.0284 (9)	0.0613 (12)	0.0427 (10)	−0.0135 (9)	0.0038 (8)	−0.0150 (9)
C15	0.0296 (11)	0.0408 (13)	0.0319 (11)	−0.0023 (10)	0.0053 (9)	−0.0044 (10)

C16	0.0216 (10)	0.0401 (12)	0.0343 (12)	−0.0010 (9)	0.0055 (9)	−0.0010 (10)

Geometric parameters (Å, º)

S1—O2	1.4286 (19)	C8—H8B	0.94 (3)
S1—O1	1.433 (2)	C8—H8A	0.95 (3)
S1—N2	1.668 (2)	C9—O9	1.226 (3)
S1—C7A	1.763 (2)	C9—N10	1.340 (3)
N2—C3	1.386 (3)	N10—C11	1.421 (3)
N2—C8	1.444 (3)	N10—H10	0.87 (3)
C3—O3	1.203 (3)	C11—C16	1.384 (3)
C3—C4A	1.484 (3)	C11—C12	1.392 (3)
C4—C4A	1.385 (3)	C12—C13	1.383 (3)
C4—C5	1.394 (4)	C12—H12	0.95 (3)
C4—H4	0.91 (3)	C13—C14	1.383 (3)
C4A—C7A	1.369 (4)	C13—H13	0.95 (3)
C5—C6	1.367 (5)	C14—O14	1.370 (3)
C5—H5	0.96 (4)	C14—C15	1.383 (3)
C6—C7	1.384 (4)	O14—H14	0.82 (3)
C6—H6	0.97 (3)	C15—C16	1.385 (3)
C7A—C7	1.377 (4)	C15—H15	0.96 (3)
C7—H7	0.93 (3)	C16—H16	0.95 (3)
C8—C9	1.522 (3)		
O2—S1—O1	117.12 (13)	N2—C8—H8B	108.3 (16)
O2—S1—N2	110.07 (11)	C9—C8—H8B	110.3 (16)
O1—S1—N2	109.35 (12)	N2—C8—H8A	106.1 (16)
O2—S1—C7A	113.30 (13)	C9—C8—H8A	109.9 (16)
O1—S1—C7A	112.41 (12)	H8B—C8—H8A	110 (2)
N2—S1—C7A	91.57 (11)	O9—C9—N10	124.6 (2)
C3—N2—C8	121.9 (2)	O9—C9—C8	122.84 (19)
C3—N2—S1	115.73 (16)	N10—C9—C8	112.52 (19)
C8—N2—S1	121.75 (17)	C9—N10—C11	128.3 (2)
O3—C3—N2	122.8 (2)	C9—N10—H10	115.0 (19)
O3—C3—C4A	128.6 (2)	C11—N10—H10	116.6 (19)
N2—C3—C4A	108.6 (2)	C16—C11—C12	119.3 (2)
C4A—C4—C5	117.2 (3)	C16—C11—N10	123.88 (19)
C4A—C4—H4	117.7 (17)	C12—C11—N10	116.8 (2)
C5—C4—H4	125.0 (17)	C13—C12—C11	120.6 (2)
C7A—C4A—C4	120.1 (2)	C13—C12—H12	121.3 (17)
C7A—C4A—C3	112.9 (2)	C11—C12—H12	117.9 (17)
C4—C4A—C3	127.0 (2)	C12—C13—C14	119.9 (2)
C6—C5—C4	121.8 (3)	C12—C13—H13	122 (2)
C6—C5—H5	120 (2)	C14—C13—H13	118 (2)
C4—C5—H5	119 (2)	O14—C14—C15	117.9 (2)
C5—C6—C7	121.2 (3)	O14—C14—C13	122.4 (2)
C5—C6—H6	120.3 (19)	C15—C14—C13	119.7 (2)
C7—C6—H6	118 (2)	C14—O14—H14	108 (2)

C4A—C7A—C7	123.2 (2)	C14—C15—C16	120.6 (2)
C4A—C7A—S1	110.83 (17)	C14—C15—H15	121.2 (16)
C7—C7A—S1	126.0 (2)	C16—C15—H15	118.1 (16)
C7A—C7—C6	116.6 (3)	C11—C16—C15	119.9 (2)
C7A—C7—H7	123 (2)	C11—C16—H16	121.3 (16)
C6—C7—H7	120 (2)	C15—C16—H16	118.8 (16)
N2—C8—C9	111.95 (19)		

O2—S1—N2—C3	121.36 (18)	O2—S1—C7A—C7	63.0 (3)
O1—S1—N2—C3	−108.64 (18)	O1—S1—C7A—C7	−72.6 (3)
C7A—S1—N2—C3	5.82 (19)	N2—S1—C7A—C7	175.7 (3)
O2—S1—N2—C8	−67.6 (2)	C4A—C7A—C7—C6	0.1 (5)
O1—S1—N2—C8	62.4 (2)	S1—C7A—C7—C6	179.4 (2)
C7A—S1—N2—C8	176.87 (19)	C5—C6—C7—C7A	−0.9 (5)
C8—N2—C3—O3	4.5 (4)	C3—N2—C8—C9	−96.0 (3)
S1—N2—C3—O3	175.5 (2)	S1—N2—C8—C9	93.5 (2)
C8—N2—C3—C4A	−176.0 (2)	N2—C8—C9—O9	6.7 (3)
S1—N2—C3—C4A	−5.0 (2)	N2—C8—C9—N10	−174.0 (2)
C5—C4—C4A—C7A	−1.1 (4)	O9—C9—N10—C11	−0.2 (4)
C5—C4—C4A—C3	177.2 (3)	C8—C9—N10—C11	−179.5 (2)
O3—C3—C4A—C7A	−179.5 (3)	C9—N10—C11—C16	6.3 (4)
N2—C3—C4A—C7A	1.0 (3)	C9—N10—C11—C12	−173.7 (2)
O3—C3—C4A—C4	2.1 (4)	C16—C11—C12—C13	0.3 (4)
N2—C3—C4A—C4	−177.4 (2)	N10—C11—C12—C13	−179.8 (2)
C4A—C4—C5—C6	0.3 (4)	C11—C12—C13—C14	0.3 (4)
C4—C5—C6—C7	0.7 (5)	C12—C13—C14—O14	179.3 (2)
C4—C4A—C7A—C7	0.9 (4)	C12—C13—C14—C15	−0.7 (4)
C3—C4A—C7A—C7	−177.6 (3)	O14—C14—C15—C16	−179.4 (2)
C4—C4A—C7A—S1	−178.4 (2)	C13—C14—C15—C16	0.6 (4)
C3—C4A—C7A—S1	3.1 (3)	C12—C11—C16—C15	−0.4 (3)
O2—S1—C7A—C4A	−117.6 (2)	N10—C11—C16—C15	179.7 (2)
O1—S1—C7A—C4A	106.8 (2)	C14—C15—C16—C11	−0.1 (4)
N2—S1—C7A—C4A	−5.0 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N10—H10···O14^{i}	0.87 (3)	2.23 (3)	3.078 (3)	165 (3)
O14—H14···O9^{ii}	0.82 (3)	1.91 (3)	2.725 (2)	173 (3)

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