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Ethyl 2-benzenesulfonamido-4-methylpentanoate

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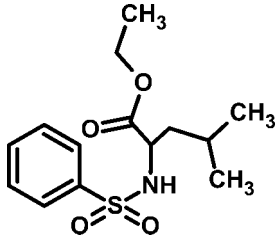
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.039; wR factor = 0.098; data-to-parameter ratio = 13.8.

In the title compound, $C_{14}H_{21}NO_4S$, the O—S—O angle is 120.06 (11)°, with the S atom adopting a distorted tetrahedral geometry. In the crystal, N—H···O hydrogen bonds connect the molecules along the a axis, generating an infinite chain. The disordered C atoms of the isobutyl group were refined with the C—C distances restrained to 1.52 (1) Å and the occupancy ratio refined to 0.504 (3):0.496 (3).

Related literature

For related structures, see: Arshad *et al.* (2010, 2012).



Experimental

Crystal data

$C_{14}H_{21}NO_4S$ M_r = 299.38
Orthorhombic, $P2_12_12_1$
a = 5.3084 (3) Å
b = 9.5507 (7) Å
c = 31.315 (2) Å
V = 1587.66 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 296 K
0.41 × 0.37 × 0.34 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.917, T_{max} = 0.930
12652 measured reflections
3081 independent reflections
2701 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.098
S = 1.04
3081 reflections
223 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}
Absolute structure: Flack (1983), 1220 Friedel pairs
Flack parameter: 0.01 (9)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.86	2.20	3.032 (2)	162

Symmetry code: (i) $x+1, y, z$.

Data collection: *APEX2* (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: *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *X-SEED* (Barbour, 2001).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5998).

References

Arshad, M. N., Danish, M., Tahir, M. N., Khalid, S. & Asiri, A. M. (2012). *Acta Cryst.* E**68**, o2573.
Arshad, M. N., Mubashar-ur-Rehman, H., Khan, I. U., Shafiq, M. & Lo, K. M. (2010). *Acta Cryst.* E**66**, o541.
Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189-191.
Bruker (2007). *SADABS*, *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

supporting information

Acta Cryst. (2012). E**68**, o2874 [https://doi.org/10.1107/S1600536812037658]

Ethyl 2-benzenesulfonamido-4-methylpentanoate

Muhammad Nadeem Arshad, Muhammad Danish, Muhammad Nawaz Tahir, Savera Khalid and Abdullah M. Asiri

S1. Comment

We report the crystal structure of title compound in continuation to our work on synthesis of sulfonamide derived from amino acids (Arshad *et al.*, 2010; Arshad *et al.*, 2012).

The methylester moiety (C7/C8/O3/O4/C9/C10) is almost planer with r. m. s. deviation of 0.0113 (2) Å and is oriented at dihedral angle of 21.37 (13)° with respect to the aromatic ring (C1—C6). The S atom adopts a distorted tetrahedral geometry and the bond angles are in comparison with the already published compound 4-methyl-2- (2-nitrobenzene-sulfonamido)pentanoic acid (Arshad *et al.*, 2012). The crystal structure shows intermolecular N—H···O hydrogen bonds connecting the molecules to a chain running along the *a* axis (Table. 1, Fig. 2). The isobutyl group is disordered over two positions with occupancies of 0.504 (3):0.496 (3) for (C11A—C14A) & (C11B—C14B) respectively.

S2. Experimental

4-Methyl-2-[(phenylsulfonyl)amino]pentanoic acid (0.20 g, 0.738 mmol) added to the mixture of NaH (0.035g, 1.47 mmol) in dimethylformamide (5 mL). The mixture was stirred for 15 mins followed by addition of ethyliodide (0.135 g, 0.86 mmol). Stirring was continued for 3-4 h and then mixture was poured on ice, precipitate obtained was filtered off, washed with water and recrystalized in ethylacetate under slow evaporation to give yellow crystal.

S3. Refinement

The early refinement showed that there are two conformations of isobutyl moiety (C11–C14). These were refined anisotropically with distance restraint and the occupancy ratio was found 0.504 (3):0.496 (3).

The H-atoms were positioned geometrically (C–H = 0.93–0.98 Å, N—H = 0.86 Å) and refined as riding with U_{iso}(H) = kU_{eq}(C, N), where k = 1.5 for methyl and k = 1.2 for all other H-atoms.

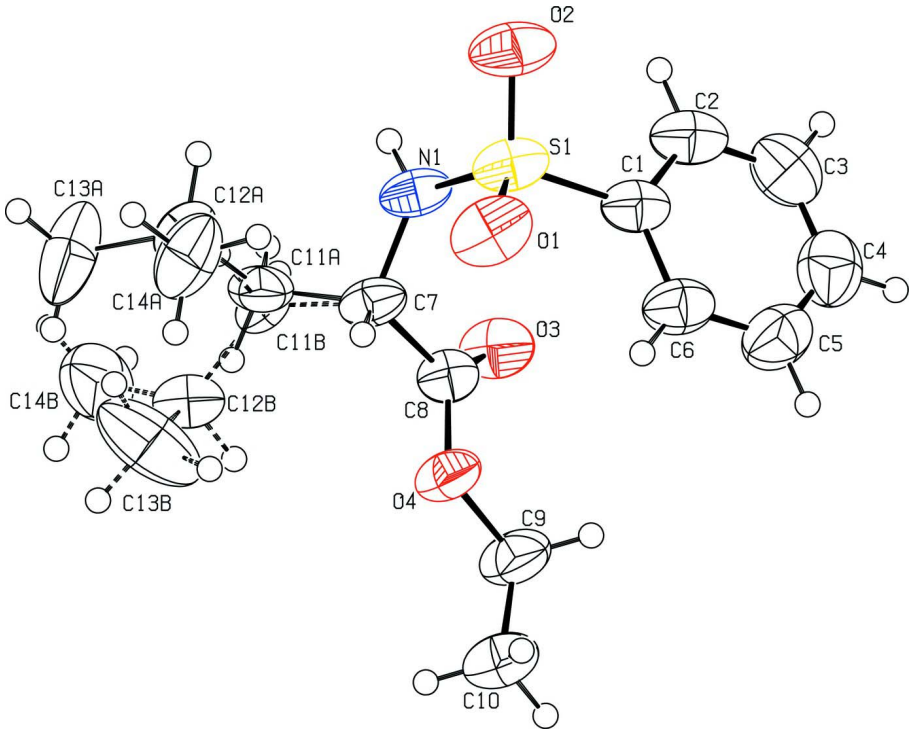

Figure 1

The labelled molecular structure of (I) with 50% displacement ellipsoids.

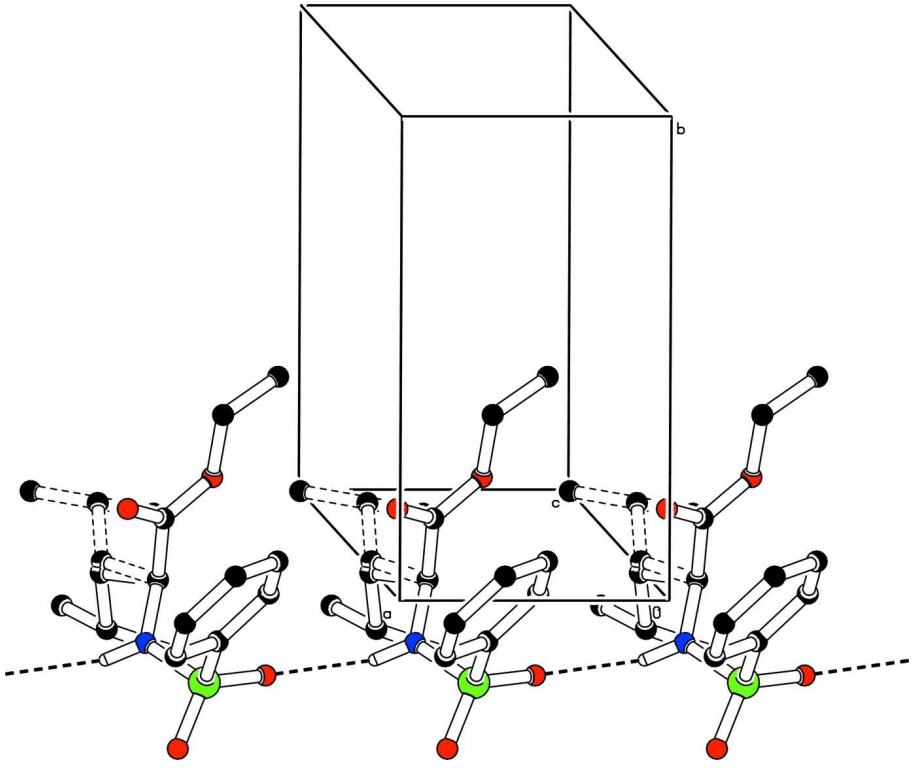

Figure 2

Unit cell packing showing hydrogen bonds, drawn using dashed lines.

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Crystal data

$C_{14}H_{21}NO_4S$
$M_r = 299.38$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 5.3084$ (3) Å
$b = 9.5507$ (7) Å
$c = 31.315$ (2) Å
$V = 1587.66$ (19) Å^3
$Z = 4$
$F(000) = 640$
$D_x = 1.252$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5078 reflections
$\theta = 2.5$–$24.4°$
$\mu = 0.22$ mm^{-1}
$T = 296$ K
Prismatic, yellow
0.41 × 0.37 × 0.34 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
$T_{min} = 0.917$, $T_{max} = 0.930$
12652 measured reflections
3081 independent reflections
2701 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.2°$
$h = -6 \rightarrow 6$
$k = -10 \rightarrow 11$
$l = -38 \rightarrow 37$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.098$
$S = 1.04$
3081 reflections
223 parameters
4 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0506P)^2 + 0.2498P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}
Absolute structure: Flack (1983), 1220 Friedel pairs
Absolute structure parameter: 0.01 (9)

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2$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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
S1	0.68578 (10)	−0.19267 (6)	0.10068 (2)	0.05767 (18)	
O1	0.4508 (3)	−0.18269 (19)	0.12304 (6)	0.0735 (5)	
O2	0.7870 (4)	−0.32649 (16)	0.09014 (6)	0.0778 (5)	
O3	0.9729 (3)	0.16642 (16)	0.09996 (6)	0.0655 (4)	
O4	0.6446 (3)	0.22241 (16)	0.14150 (5)	0.0570 (4)	
N1	0.8935 (3)	−0.11735 (19)	0.13029 (6)	0.0536 (5)	
H1	1.0426	−0.1524	0.1315	0.064*	
C1	0.6547 (4)	−0.0963 (2)	0.05333 (7)	0.0527 (5)	
C2	0.8230 (5)	−0.1196 (3)	0.02036 (9)	0.0683 (7)	
H2	0.9491	−0.1866	0.0232	0.082*	
C3	0.8025 (6)	−0.0431 (3)	−0.01669 (9)	0.0783 (8)	
H3	0.9157	−0.0582	−0.0389	0.094*	
C4	0.6176 (6)	0.0547 (3)	−0.02112 (9)	0.0784 (8)	
H4	0.6048	0.1058	−0.0463	0.094*	
C5	0.4501 (6)	0.0782 (3)	0.01152 (9)	0.0757 (8)	
H5	0.3238	0.1448	0.0083	0.091*	
C6	0.4679 (5)	0.0031 (2)	0.04935 (9)	0.0626 (6)	
H6	0.3558	0.0195	0.0716	0.075*	
C7	0.8389 (4)	0.0075 (2)	0.15512 (7)	0.0510 (5)	
H7A	0.6742	−0.0049	0.1687	0.061*	0.504 (3)
H7B	0.6744	−0.0049	0.1688	0.061*	0.496 (3)
C8	0.8294 (4)	0.1402 (2)	0.12817 (7)	0.0478 (5)	
C9	0.6135 (5)	0.3561 (3)	0.11924 (8)	0.0707 (7)	
H9A	0.5766	0.3403	0.0893	0.085*	
H9B	0.7665	0.4112	0.1213	0.085*	
C10	0.4024 (5)	0.4301 (3)	0.13998 (9)	0.0724 (7)	
H10A	0.2535	0.3732	0.1385	0.109*	
H10B	0.3728	0.5173	0.1256	0.109*	
H10C	0.4434	0.4478	0.1693	0.109*	
C11A	1.0382 (19)	0.0138 (11)	0.1901 (3)	0.060 (3)	0.504 (3)
H11A	1.2049	0.0103	0.1775	0.072*	0.504 (3)
H11B	1.0227	0.1010	0.2058	0.072*	0.504 (3)
C12A	1.0033 (10)	−0.1090 (5)	0.22027 (16)	0.0621 (13)	0.504 (3)
H12A	1.0898	−0.1889	0.2072	0.074*	0.504 (3)
C13A	1.1548 (15)	−0.0698 (8)	0.2604 (2)	0.109 (3)	0.504 (3)
H13A	1.3229	−0.0439	0.2522	0.164*	0.504 (3)
H13B	1.1612	−0.1486	0.2793	0.164*	0.504 (3)
H13C	1.0751	0.0076	0.2745	0.164*	0.504 (3)
C14A	0.7472 (11)	−0.1593 (7)	0.23266 (19)	0.088 (2)	0.504 (3)
H14A	0.6591	−0.1909	0.2077	0.131*	0.504 (3)
H14B	0.6551	−0.0840	0.2457	0.131*	0.504 (3)
H14C	0.7628	−0.2351	0.2526	0.131*	0.504 (3)
C11B	1.034 (3)	0.0378 (12)	0.1901 (3)	0.075 (4)	0.496 (3)
H11C	1.0500	−0.0496	0.2056	0.090*	0.496 (3)
H11D	1.1919	0.0496	0.1748	0.090*	0.496 (3)

C12B	1.0376 (9)	0.1504 (5)	0.22429 (16)	0.0629 (14)	0.496 (3)
H12B	1.0034	0.2396	0.2100	0.076*	0.496 (3)
C13B	0.8197 (16)	0.1219 (9)	0.2529 (2)	0.123 (3)	0.496 (3)
H13D	0.6658	0.1310	0.2370	0.185*	0.496 (3)
H13E	0.8201	0.1877	0.2761	0.185*	0.496 (3)
H13F	0.8327	0.0285	0.2640	0.185*	0.496 (3)
C14B	1.2773 (13)	0.1690 (8)	0.2491 (2)	0.099 (2)	0.496 (3)
H14D	1.4122	0.1911	0.2298	0.149*	0.496 (3)
H14E	1.3159	0.0840	0.2640	0.149*	0.496 (3)
H14F	1.2570	0.2439	0.2692	0.149*	0.496 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0400 (3)	0.0384 (3)	0.0946 (4)	−0.0045 (2)	0.0071 (3)	0.0040 (3)
O1	0.0384 (8)	0.0736 (12)	0.1084 (13)	−0.0082 (8)	0.0124 (8)	0.0184 (11)
O2	0.0729 (11)	0.0343 (9)	0.1263 (15)	−0.0015 (8)	0.0013 (11)	−0.0036 (9)
O3	0.0647 (10)	0.0535 (10)	0.0784 (10)	−0.0005 (8)	0.0242 (9)	0.0123 (8)
O4	0.0584 (9)	0.0451 (8)	0.0674 (9)	0.0129 (8)	0.0097 (8)	0.0148 (7)
N1	0.0340 (9)	0.0432 (10)	0.0836 (12)	0.0074 (8)	0.0088 (9)	0.0030 (9)
C1	0.0395 (11)	0.0409 (11)	0.0778 (14)	−0.0056 (9)	0.0017 (11)	−0.0087 (10)
C2	0.0552 (13)	0.0550 (14)	0.0947 (18)	0.0057 (13)	0.0089 (15)	−0.0115 (13)
C3	0.0778 (18)	0.085 (2)	0.0726 (16)	−0.0104 (19)	0.0109 (16)	−0.0110 (15)
C4	0.080 (2)	0.082 (2)	0.0730 (16)	−0.0125 (17)	−0.0117 (15)	0.0004 (15)
C5	0.0655 (16)	0.0669 (17)	0.0948 (19)	0.0050 (14)	−0.0179 (15)	0.0024 (15)
C6	0.0457 (13)	0.0556 (14)	0.0865 (17)	0.0043 (11)	0.0018 (12)	−0.0048 (13)
C7	0.0421 (11)	0.0433 (12)	0.0675 (12)	0.0079 (11)	0.0164 (10)	0.0092 (10)
C8	0.0422 (10)	0.0406 (11)	0.0606 (11)	−0.0042 (10)	0.0028 (11)	0.0013 (9)
C9	0.0836 (19)	0.0505 (13)	0.0781 (15)	0.0187 (13)	0.0113 (14)	0.0189 (12)
C10	0.0731 (17)	0.0505 (14)	0.0934 (18)	0.0137 (13)	0.0052 (15)	0.0107 (13)
C11A	0.086 (6)	0.036 (4)	0.057 (5)	0.014 (3)	0.016 (4)	0.002 (3)
C12A	0.061 (3)	0.054 (3)	0.071 (3)	0.005 (2)	−0.006 (2)	0.015 (2)
C13A	0.115 (6)	0.112 (5)	0.101 (4)	−0.035 (5)	−0.060 (5)	0.047 (4)
C14A	0.076 (4)	0.102 (5)	0.084 (4)	−0.003 (3)	−0.003 (3)	0.043 (3)
C11B	0.120 (9)	0.044 (5)	0.060 (6)	0.028 (5)	−0.023 (5)	0.008 (4)
C12B	0.058 (3)	0.051 (3)	0.080 (3)	0.007 (2)	0.008 (3)	−0.003 (2)
C13B	0.104 (5)	0.140 (7)	0.126 (6)	−0.042 (6)	0.058 (5)	−0.068 (5)
C14B	0.080 (4)	0.120 (6)	0.097 (4)	0.007 (4)	−0.023 (3)	−0.033 (4)

Geometric parameters (Å, º)

S1—O2	1.4251 (17)	C10—H10A	0.9600
S1—O1	1.4336 (16)	C10—H10B	0.9600
S1—N1	1.6104 (19)	C10—H10C	0.9600
S1—C1	1.753 (2)	C11A—C12A	1.517 (9)
O3—C8	1.193 (2)	C11A—H11A	0.9700
O4—C8	1.324 (3)	C11A—H11B	0.9700
O4—C9	1.464 (3)	C12A—C14A	1.493 (8)

N1—C7	1.453 (3)	C12A—C13A	1.537 (7)
N1—H1	0.8600	C12A—H12A	0.9800
C1—C6	1.378 (3)	C13A—H13A	0.9600
C1—C2	1.383 (3)	C13A—H13B	0.9600
C2—C3	1.376 (4)	C13A—H13C	0.9600
C2—H2	0.9300	C14A—H14A	0.9600
C3—C4	1.362 (4)	C14A—H14B	0.9600
C3—H3	0.9300	C14A—H14C	0.9600
C4—C5	1.373 (4)	C11B—C12B	1.519 (9)
C4—H4	0.9300	C11B—H11C	0.9700
C5—C6	1.388 (4)	C11B—H11D	0.9700
C5—H5	0.9300	C12B—C13B	1.488 (8)
C6—H6	0.9300	C12B—C14B	1.501 (8)
C7—C8	1.523 (3)	C12B—H12B	0.9800
C7—C11A	1.524 (7)	C13B—H13D	0.9600
C7—C11B	1.535 (8)	C13B—H13E	0.9600
C7—H7A	0.9800	C13B—H13F	0.9600
C7—H7B	0.9800	C14B—H14D	0.9600
C9—C10	1.475 (4)	C14B—H14E	0.9600
C9—H9A	0.9700	C14B—H14F	0.9600
C9—H9B	0.9700		

O2—S1—O1	120.06 (11)	O4—C9—H9A	110.3
O2—S1—N1	106.01 (10)	C10—C9—H9A	110.3
O1—S1—N1	106.54 (11)	O4—C9—H9B	110.3
O2—S1—C1	108.08 (11)	C10—C9—H9B	110.3
O1—S1—C1	107.24 (11)	H9A—C9—H9B	108.6
N1—S1—C1	108.49 (10)	C9—C10—H10A	109.5
C8—O4—C9	116.81 (17)	C9—C10—H10B	109.5
C7—N1—S1	122.57 (14)	H10A—C10—H10B	109.5
C7—N1—H1	118.7	C9—C10—H10C	109.5
S1—N1—H1	118.7	H10A—C10—H10C	109.5
C6—C1—C2	120.5 (2)	H10B—C10—H10C	109.5
C6—C1—S1	120.38 (18)	C12A—C11A—C7	109.4 (6)
C2—C1—S1	119.06 (18)	C12A—C11A—H11A	109.8
C3—C2—C1	119.5 (3)	C7—C11A—H11A	109.8
C3—C2—H2	120.3	C12A—C11A—H11B	109.8
C1—C2—H2	120.3	C7—C11A—H11B	109.8
C4—C3—C2	120.5 (3)	H11A—C11A—H11B	108.2
C4—C3—H3	119.7	C14A—C12A—C11A	121.4 (5)
C2—C3—H3	119.7	C14A—C12A—C13A	110.0 (5)
C3—C4—C5	120.2 (3)	C11A—C12A—C13A	104.9 (5)
C3—C4—H4	119.9	C14A—C12A—H12A	106.5
C5—C4—H4	119.9	C11A—C12A—H12A	106.5
C4—C5—C6	120.5 (3)	C13A—C12A—H12A	106.5
C4—C5—H5	119.8	C12B—C11B—C7	130.2 (8)
C6—C5—H5	119.8	C12B—C11B—H11C	104.7
C1—C6—C5	118.8 (2)	C7—C11B—H11C	104.7

C1—C6—H6	120.6	C12B—C11B—H11D	104.7
C5—C6—H6	120.6	C7—C11B—H11D	104.7
N1—C7—C8	113.15 (17)	H11C—C11B—H11D	105.7
N1—C7—C11A	106.2 (5)	C13B—C12B—C14B	111.7 (5)
C8—C7—C11A	112.9 (4)	C13B—C12B—C11B	106.6 (7)
N1—C7—C11B	113.7 (5)	C14B—C12B—C11B	117.3 (6)
C8—C7—C11B	105.1 (5)	C13B—C12B—H12B	106.9
C11A—C7—C11B	8.6 (8)	C14B—C12B—H12B	106.9
N1—C7—H7A	108.2	C11B—C12B—H12B	106.9
C8—C7—H7A	108.2	C12B—C13B—H13D	109.5
C11A—C7—H7A	108.2	C12B—C13B—H13E	109.5
C11B—C7—H7A	108.4	H13D—C13B—H13E	109.5
N1—C7—H7B	108.2	C12B—C13B—H13F	109.5
C8—C7—H7B	108.2	H13D—C13B—H13F	109.5
C11A—C7—H7B	108.0	H13E—C13B—H13F	109.5
C11B—C7—H7B	108.2	C12B—C14B—H14D	109.5
H7A—C7—H7B	0.2	C12B—C14B—H14E	109.5
O3—C8—O4	125.57 (19)	H14D—C14B—H14E	109.5
O3—C8—C7	124.3 (2)	C12B—C14B—H14F	109.5
O4—C8—C7	110.08 (17)	H14D—C14B—H14F	109.5
O4—C9—C10	107.1 (2)	H14E—C14B—H14F	109.5

O2—S1—N1—C7	−166.24 (16)	C9—O4—C8—O3	0.7 (3)
O1—S1—N1—C7	−37.29 (19)	C9—O4—C8—C7	178.89 (19)
C1—S1—N1—C7	77.88 (18)	N1—C7—C8—O3	−41.0 (3)
O2—S1—C1—C6	150.11 (18)	C11A—C7—C8—O3	79.6 (5)
O1—S1—C1—C6	19.3 (2)	C11B—C7—C8—O3	83.6 (6)
N1—S1—C1—C6	−95.37 (19)	N1—C7—C8—O4	140.70 (18)
O2—S1—C1—C2	−31.1 (2)	C11A—C7—C8—O4	−98.7 (5)
O1—S1—C1—C2	−161.86 (19)	C11B—C7—C8—O4	−94.7 (6)
N1—S1—C1—C2	83.4 (2)	C8—O4—C9—C10	−178.8 (2)
C6—C1—C2—C3	−0.2 (4)	N1—C7—C11A—C12A	−65.9 (7)
S1—C1—C2—C3	−179.0 (2)	C8—C7—C11A—C12A	169.6 (5)
C1—C2—C3—C4	−0.2 (4)	C11B—C7—C11A—C12A	143 (7)
C2—C3—C4—C5	0.2 (4)	C7—C11A—C12A—C14A	−38.3 (10)
C3—C4—C5—C6	0.3 (4)	C7—C11A—C12A—C13A	−163.6 (7)
C2—C1—C6—C5	0.7 (3)	N1—C7—C11B—C12B	−175.5 (10)
S1—C1—C6—C5	179.49 (19)	C8—C7—C11B—C12B	60.3 (13)
C4—C5—C6—C1	−0.7 (4)	C11A—C7—C11B—C12B	−145 (7)
S1—N1—C7—C8	−76.4 (2)	C7—C11B—C12B—C13B	64.6 (14)
S1—N1—C7—C11A	159.2 (4)	C7—C11B—C12B—C14B	−169.4 (10)
S1—N1—C7—C11B	163.8 (6)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.86	2.20	3.032 (2)	162

Symmetry code: (i) $x+1, y, z$.