



ISSN 2414-3146

# (E)-N-[Cyclopentyl(morpholin-4-yl)methylidene]-4-fluorobenzenesulfonamide

Ilya Efimov,<sup>a\*</sup> Pavel Slepukhin,<sup>b</sup> Nikolai Beliaev<sup>a</sup> and Vasilii Bakulev<sup>a</sup><sup>a</sup>Ural Federal University, Mira 19 Ekaterinburg 620002, Russian Federation, and <sup>b</sup>I. Ya. Postovsky Institute of Organic Synthesis, Ural Branch of Russian Academy, of Sciences, 20 S. Kovalevskaya str., 620990 Ekaterinburg, Russia.

\*Correspondence e-mail: aspirant\_efimov@mail.ru

Received 17 December 2015

Accepted 4 January 2016

Edited by W. T. A. Harrison, University of Aberdeen, Scotland

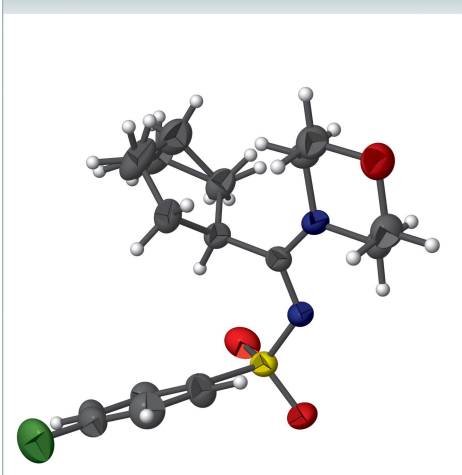
Keywords: crystal structure; amidines; transformation.

CCDC reference: 1445312

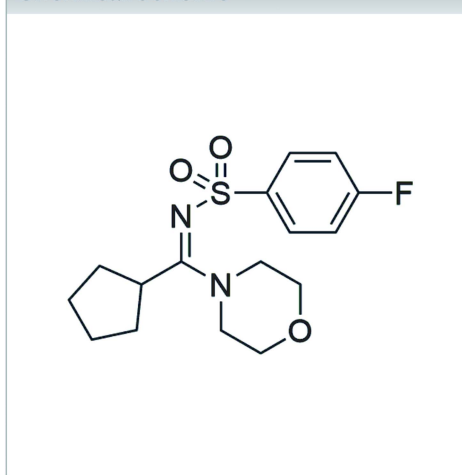
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, C<sub>16</sub>H<sub>21</sub>FN<sub>2</sub>O<sub>3</sub>S, was obtained from the reaction between sulfonyl azide, cyclohexanone and morpholine. The bond lengths at the amidine N—C—N grouping are similar [1.326 (3) and 1.338 (3) Å], indicating significant conjugation. The cyclopentyl moiety displays disorder of one of the methylene groups into two orientations with occupancy coefficients 0.75/0.25. No shortened intermolecular contacts in the crystal are observed.

## 3D view



## Chemical scheme



## Structure description

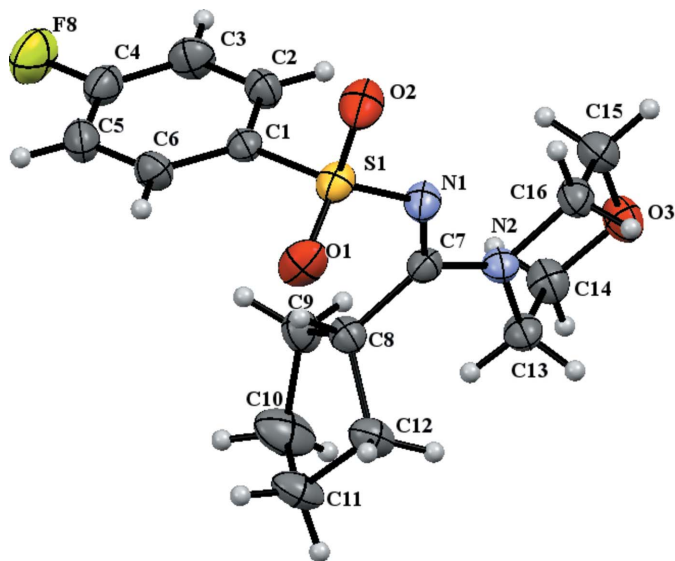
The title compound is illustrated in Fig. 1. For background to sulfonamides, see: Xu *et al.* (2008); Xie *et al.* (2015).

## Synthesis and crystallization

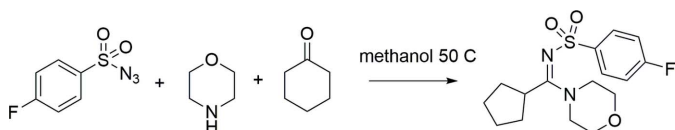
In a 10-ml tube with a stirring bar, 4-fluorobenzene-1-sulfonyl azide (1 mmol, 201 mg), cyclohexanone (2 mmol, 206 ml), morpholine (2 mmol, 173 ml) and 2 ml methanol were added successively; the mixture was then stirred at room temperature. After cooling down, the volatiles were removed under reduced pressure (Fig. 2). To the residue was added 5% water solution of CH<sub>3</sub>COOH and mixture was stirred over 2 h. The resulting precipitate was filtered off, washed with water, dried and recrystallized from water.

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.



**Figure 1**  
The title compound.



**Figure 2**  
Reaction scheme.

## Acknowledgements

This work was supported by RFBR (14-03-01033).

## References

- Agilent (2013). *CrysAlis PRO*. Agilent Technologies Ltd, Yarnton, England.  
 Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.

**Table 1**  
Experimental details.

Crystal data	
Chemical formula	C <sub>16</sub> H <sub>21</sub> FN <sub>2</sub> O <sub>3</sub> S
<i>M<sub>r</sub></i>	340.41
Crystal system, space group	Monoclinic, <i>P</i> 2 <sub>1</sub> / <i>c</i>
Temperature (K)	295
<i>a</i> , <i>b</i> , <i>c</i> (Å)	11.5613 (7), 16.4245 (13), 8.8730 (6)
$\beta$ (°)	107.768 (6)
<i>V</i> (Å <sup>3</sup> )	1604.5 (2)
<i>Z</i>	4
Radiation type	Mo <i>K</i> $\alpha$
$\mu$ (mm <sup>-1</sup> )	0.23
Crystal size (mm)	0.25 × 0.17 × 0.03
Data collection	
Diffractometer	Agilent Xcalibur, Eos diffractometer
Absorption correction	Multi-scan ( <i>CrysAlis PRO</i> ; Agilent, 2013)
<i>T<sub>min</sub></i> , <i>T<sub>max</sub></i>	0.939, 1.000
No. of measured, independent and observed [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )] reflections	6974, 3391, 2323
<i>R<sub>int</sub></i>	0.029
( <i>sin</i> $\theta$ / $\lambda$ ) <sub>max</sub> (Å <sup>-1</sup> )	0.641
Refinement	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2 $\sigma$ ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.046, 0.137, 1.01
No. of reflections	3391
No. of parameters	221
No. of restraints	6
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\max}$ , $\Delta\rho_{\min}$ (e Å <sup>-3</sup> )	0.29, -0.38

Computer programs: *CrysAlis PRO* (Agilent, 2013), *SHELXS* (Sheldrick, 2008), *SHELXL* (Sheldrick, 2008), *OLEX2* (Dolomanov *et al.*, 2009).

- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
 Xie, S., Lopez, S. A., Ramström, O., Yan, M. & Houk, K. N. (2015). *J. Am. Chem. Soc.* **137**, 2958–2966.  
 Xu, X., Li, X., Ma, L., Ye, N. & Weng, B. (2008). *J. Am. Chem. Soc.* **130**, 14048–14049.

## full crystallographic data

*IUCrData* (2016). **1**, x160013 [doi:10.1107/S2414314616000134]

**(*E*)-*N*-[Cyclopentyl(morpholin-4-yl)methylidene]-4-fluorobenzenesulfonamide**

Ilya Efimov, Pavel Slepukhin, Nikolai Beliaev and Vasiliy Bakulev

**(*E*)-*N*-[Cyclopentyl(morpholin-4-yl)methylidene]-4-fluorobenzenesulfonamide***Crystal data*

$C_{16}H_{21}FN_2O_3S$

$M_r = 340.41$

Monoclinic,  $P2_1/c$

$a = 11.5613$  (7) Å

$b = 16.4245$  (13) Å

$c = 8.8730$  (6) Å

$\beta = 107.768$  (6)°

$V = 1604.5$  (2) Å<sup>3</sup>

$Z = 4$

$F(000) = 720$

$D_x = 1.409$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.7107$  Å

Cell parameters from 1405 reflections

$\theta = 2.8$ – $27.0$ °

$\mu = 0.23$  mm<sup>-1</sup>

$T = 295$  K

Plank, colourless

$0.25 \times 0.17 \times 0.03$  mm

*Data collection*

Agilent Xcalibur, Eos  
diffractometer

Radiation source: Enhance (Mo) X-ray Source  
Graphite monochromator

Detector resolution: 15.9555 pixels mm<sup>-1</sup>  
 $\omega$  scans

Absorption correction: multi-scan  
(*CrysAlis PRO*; Agilent, 2013)

$T_{\min} = 0.939$ ,  $T_{\max} = 1.000$

6974 measured reflections

3391 independent reflections

2323 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.029$

$\theta_{\max} = 27.1$ °,  $\theta_{\min} = 2.2$ °

$h = -9 \rightarrow 14$

$k = -21 \rightarrow 18$

$l = -10 \rightarrow 11$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.046$

$wR(F^2) = 0.137$

$S = 1.01$

3391 reflections

221 parameters

6 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

$w = 1/[\sigma^2(F_o^2) + (0.075P)^2 + 0.010P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.29$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.38$  e Å<sup>-3</sup>

*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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
S1	0.26452 (5)	0.09127 (4)	0.07277 (6)	0.04217 (19)	
N2	0.45896 (15)	0.09749 (12)	-0.20031 (19)	0.0369 (4)	
N1	0.37106 (15)	0.10138 (13)	-0.0054 (2)	0.0413 (5)	
C1	0.14033 (18)	0.14851 (14)	-0.0468 (2)	0.0347 (5)	
C7	0.36523 (18)	0.07661 (14)	-0.1498 (2)	0.0352 (5)	
O1	0.22350 (16)	0.00860 (11)	0.07573 (19)	0.0568 (5)	
C8	0.26032 (19)	0.02854 (15)	-0.2575 (2)	0.0381 (5)	
O3	0.60684 (14)	0.19090 (11)	-0.33829 (19)	0.0528 (5)	
F8	-0.14638 (14)	0.28150 (12)	-0.3150 (2)	0.0788 (5)	
C2	0.1600 (2)	0.22178 (15)	-0.1115 (3)	0.0444 (6)	
H2	0.2388	0.2406	-0.0946	0.053*	
O2	0.30637 (15)	0.13122 (13)	0.22357 (18)	0.0605 (5)	
C13	0.4793 (2)	0.07269 (15)	-0.3481 (2)	0.0419 (6)	
H13A	0.4078	0.0450	-0.4148	0.050*	
H13B	0.5472	0.0351	-0.3259	0.050*	
C3	0.0632 (2)	0.26682 (16)	-0.2006 (3)	0.0523 (6)	
H3	0.0754	0.3165	-0.2437	0.063*	
C4	-0.0514 (2)	0.23724 (17)	-0.2248 (3)	0.0498 (6)	
C16	0.56120 (19)	0.14650 (16)	-0.1027 (3)	0.0437 (6)	
H16A	0.6336	0.1130	-0.0675	0.052*	
H16B	0.5425	0.1665	-0.0099	0.052*	
C14	0.5058 (2)	0.14643 (17)	-0.4328 (3)	0.0489 (6)	
H14A	0.5216	0.1293	-0.5292	0.059*	
H14B	0.4350	0.1815	-0.4621	0.059*	
C5	-0.0748 (2)	0.16534 (17)	-0.1626 (3)	0.0503 (6)	
H5	-0.1541	0.1472	-0.1801	0.060*	
C9	0.1918 (2)	0.06850 (17)	-0.4184 (3)	0.0490 (6)	
H9A	0.1177	0.0946	-0.4135	0.059*	
H9B	0.2424	0.1088	-0.4477	0.059*	
C6	0.0229 (2)	0.12052 (15)	-0.0730 (3)	0.0446 (6)	
H6	0.0097	0.0711	-0.0298	0.053*	
C12	0.2895 (2)	-0.05923 (15)	-0.2949 (3)	0.0490 (6)	
H12A	0.3680	-0.0622	-0.3131	0.059*	0.75
H12B	0.2890	-0.0960	-0.2096	0.059*	0.75
H12C	0.2512	-0.0983	-0.2434	0.059*	0.25
H12D	0.3765	-0.0687	-0.2607	0.059*	0.25
C15	0.5838 (2)	0.21732 (16)	-0.1983 (3)	0.0509 (6)	
H15A	0.5135	0.2529	-0.2260	0.061*	
H15B	0.6528	0.2484	-0.1346	0.061*	
C11	0.1861 (5)	-0.0793 (3)	-0.4464 (5)	0.0564 (12)	0.75

H11A	0.2104	-0.1217	-0.5066	0.068*	0.75
H11B	0.1141	-0.0970	-0.4213	0.068*	0.75
C10	0.1633 (3)	-0.0017 (2)	-0.5361 (3)	0.0769 (10)	
H10A	0.0791	0.0011	-0.6013	0.092*	0.75
H10B	0.2143	0.0016	-0.6047	0.092*	0.75
H10C	0.0791	-0.0179	-0.5574	0.092*	0.25
H10D	0.1749	0.0157	-0.6350	0.092*	0.25
H8	0.2026 (19)	0.0260 (13)	-0.203 (2)	0.032 (5)*	
C11A	0.2368 (14)	-0.0656 (11)	-0.477 (2)	0.067 (4)	0.25
H11C	0.3027	-0.0669	-0.5232	0.081*	0.25
H11D	0.1912	-0.1159	-0.5047	0.081*	0.25

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S1	0.0421 (3)	0.0542 (4)	0.0311 (3)	0.0068 (3)	0.0124 (2)	0.0008 (2)
N2	0.0384 (9)	0.0416 (12)	0.0318 (10)	-0.0014 (8)	0.0121 (7)	-0.0063 (8)
N1	0.0360 (9)	0.0565 (14)	0.0311 (10)	0.0024 (9)	0.0099 (7)	-0.0061 (8)
C1	0.0356 (11)	0.0384 (13)	0.0321 (11)	-0.0013 (9)	0.0135 (8)	-0.0051 (9)
C7	0.0350 (11)	0.0366 (13)	0.0336 (12)	0.0057 (9)	0.0099 (8)	-0.0001 (8)
O1	0.0676 (11)	0.0494 (12)	0.0606 (11)	0.0099 (9)	0.0305 (9)	0.0175 (8)
C8	0.0383 (12)	0.0427 (14)	0.0342 (12)	-0.0046 (10)	0.0124 (9)	-0.0024 (9)
O3	0.0478 (9)	0.0614 (12)	0.0509 (10)	-0.0124 (8)	0.0176 (7)	-0.0003 (8)
F8	0.0623 (10)	0.0796 (14)	0.0833 (11)	0.0288 (9)	0.0054 (8)	0.0109 (9)
C2	0.0377 (12)	0.0426 (15)	0.0527 (14)	-0.0070 (11)	0.0135 (10)	-0.0003 (11)
O2	0.0537 (10)	0.0952 (16)	0.0311 (9)	0.0093 (10)	0.0106 (7)	-0.0109 (9)
C13	0.0428 (12)	0.0485 (15)	0.0371 (13)	-0.0021 (10)	0.0162 (9)	-0.0069 (10)
C3	0.0590 (15)	0.0397 (15)	0.0577 (15)	0.0003 (12)	0.0170 (11)	0.0082 (11)
C4	0.0426 (13)	0.0547 (17)	0.0475 (14)	0.0131 (12)	0.0067 (10)	-0.0051 (11)
C16	0.0362 (11)	0.0535 (16)	0.0389 (12)	-0.0028 (11)	0.0077 (9)	-0.0074 (10)
C14	0.0480 (13)	0.0581 (18)	0.0406 (13)	-0.0057 (12)	0.0134 (10)	0.0014 (11)
C5	0.0351 (12)	0.0601 (19)	0.0543 (15)	-0.0031 (11)	0.0115 (10)	-0.0075 (12)
C9	0.0433 (13)	0.0505 (16)	0.0457 (14)	-0.0002 (11)	0.0024 (10)	0.0003 (11)
C6	0.0445 (12)	0.0390 (14)	0.0526 (14)	-0.0074 (11)	0.0183 (10)	-0.0017 (10)
C12	0.0586 (15)	0.0392 (15)	0.0426 (14)	-0.0036 (12)	0.0059 (10)	0.0004 (10)
C15	0.0482 (13)	0.0498 (17)	0.0525 (15)	-0.0062 (12)	0.0120 (11)	-0.0074 (12)
C11	0.072 (3)	0.045 (2)	0.041 (2)	-0.013 (2)	0.0011 (19)	-0.0076 (16)
C10	0.097 (2)	0.069 (2)	0.0436 (16)	-0.0073 (19)	-0.0093 (14)	-0.0045 (13)
C11A	0.070 (8)	0.056 (7)	0.066 (7)	-0.004 (6)	0.007 (6)	-0.012 (6)

*Geometric parameters (Å, °)*

S1—N1	1.5963 (19)	C16—C15	1.509 (4)
S1—C1	1.772 (2)	C14—H14A	0.9700
S1—O1	1.4412 (19)	C14—H14B	0.9700
S1—O2	1.4352 (17)	C5—H5	0.9300
N2—C7	1.338 (3)	C5—C6	1.379 (3)
N2—C13	1.459 (3)	C9—H9A	0.9700

N2—C16	1.473 (3)	C9—H9B	0.9700
N1—C7	1.326 (3)	C9—C10	1.523 (4)
C1—C2	1.382 (3)	C6—H6	0.9300
C1—C6	1.385 (3)	C12—H12A	0.9700
C7—C8	1.517 (3)	C12—H12B	0.9700
C8—C9	1.551 (3)	C12—H12C	0.9700
C8—C12	1.540 (3)	C12—H12D	0.9700
C8—H8	0.94 (2)	C12—C11	1.537 (5)
O3—C14	1.415 (3)	C12—C11A	1.545 (17)
O3—C15	1.416 (3)	C15—H15A	0.9700
F8—C4	1.356 (3)	C15—H15B	0.9700
C2—H2	0.9300	C11—H11A	0.9700
C2—C3	1.373 (3)	C11—H11B	0.9700
C13—H13A	0.9700	C11—C10	1.483 (5)
C13—H13B	0.9700	C10—H10A	0.9700
C13—C14	1.505 (3)	C10—H10B	0.9700
C3—H3	0.9300	C10—H10C	0.9700
C3—C4	1.365 (3)	C10—H10D	0.9700
C4—C5	1.365 (4)	C10—C11A	1.353 (17)
C16—H16A	0.9700	C11A—H11C	0.9700
C16—H16B	0.9700	C11A—H11D	0.9700
N1—S1—C1	106.04 (10)	C5—C6—H6	119.7
O1—S1—N1	114.06 (11)	C8—C12—H12A	111.2
O1—S1—C1	107.44 (10)	C8—C12—H12B	111.2
O2—S1—N1	105.80 (10)	C8—C12—H12C	110.9
O2—S1—C1	107.26 (11)	C8—C12—H12D	110.9
O2—S1—O1	115.66 (12)	C8—C12—C11A	104.3 (7)
C7—N2—C13	126.79 (18)	H12A—C12—H12B	109.1
C7—N2—C16	121.98 (18)	H12A—C12—H12C	129.0
C13—N2—C16	111.13 (17)	H12A—C12—H12D	27.3
C7—N1—S1	124.71 (16)	H12B—C12—H12C	26.8
C2—C1—S1	120.31 (16)	H12B—C12—H12D	84.7
C2—C1—C6	119.8 (2)	H12C—C12—H12D	108.9
C6—C1—S1	119.90 (18)	C11—C12—C8	103.1 (2)
N2—C7—C8	119.76 (18)	C11—C12—H12A	111.2
N1—C7—N2	115.94 (19)	C11—C12—H12B	111.2
N1—C7—C8	124.3 (2)	C11—C12—H12C	85.7
C7—C8—C9	116.42 (19)	C11—C12—H12D	134.0
C7—C8—C12	115.96 (18)	C11—C12—C11A	28.2 (5)
C7—C8—H8	105.0 (12)	C11A—C12—H12A	85.0
C9—C8—H8	104.4 (12)	C11A—C12—H12B	132.7
C12—C8—C9	106.34 (18)	C11A—C12—H12C	110.9
C12—C8—H8	107.9 (14)	C11A—C12—H12D	110.9
C14—O3—C15	109.61 (17)	O3—C15—C16	111.6 (2)
C1—C2—H2	120.0	O3—C15—H15A	109.3
C3—C2—C1	120.0 (2)	O3—C15—H15B	109.3
C3—C2—H2	120.0	C16—C15—H15A	109.3

N2—C13—H13A	109.7	C16—C15—H15B	109.3
N2—C13—H13B	109.7	H15A—C15—H15B	108.0
N2—C13—C14	109.7 (2)	C12—C11—H11A	110.9
H13A—C13—H13B	108.2	C12—C11—H11B	110.9
C14—C13—H13A	109.7	H11A—C11—H11B	108.9
C14—C13—H13B	109.7	C10—C11—C12	104.4 (3)
C2—C3—H3	120.6	C10—C11—H11A	110.9
C4—C3—C2	118.7 (2)	C10—C11—H11B	110.9
C4—C3—H3	120.6	C9—C10—H10A	110.0
F8—C4—C3	118.3 (3)	C9—C10—H10B	110.0
F8—C4—C5	118.5 (2)	C9—C10—H10C	109.7
C3—C4—C5	123.2 (2)	C9—C10—H10D	109.7
N2—C16—H16A	109.7	C11—C10—C9	108.5 (3)
N2—C16—H16B	109.7	C11—C10—H10A	110.0
N2—C16—C15	109.63 (18)	C11—C10—H10B	110.0
H16A—C16—H16B	108.2	C11—C10—H10C	82.6
C15—C16—H16A	109.7	C11—C10—H10D	133.4
C15—C16—H16B	109.7	H10A—C10—H10B	108.4
O3—C14—C13	112.12 (18)	H10A—C10—H10C	29.8
O3—C14—H14A	109.2	H10A—C10—H10D	80.6
O3—C14—H14B	109.2	H10B—C10—H10C	131.2
C13—C14—H14A	109.2	H10B—C10—H10D	30.4
C13—C14—H14B	109.2	H10C—C10—H10D	108.2
H14A—C14—H14B	107.9	C11A—C10—C9	110.0 (7)
C4—C5—H5	121.1	C11A—C10—C11	30.3 (7)
C4—C5—C6	117.8 (2)	C11A—C10—H10A	131.7
C6—C5—H5	121.1	C11A—C10—H10B	81.7
C8—C9—H9A	110.8	C11A—C10—H10C	109.7
C8—C9—H9B	110.8	C11A—C10—H10D	109.7
H9A—C9—H9B	108.9	C12—C11A—H11C	109.5
C10—C9—C8	104.7 (2)	C12—C11A—H11D	109.5
C10—C9—H9A	110.8	C10—C11A—C12	110.7 (11)
C10—C9—H9B	110.8	C10—C11A—H11C	109.5
C1—C6—H6	119.7	C10—C11A—H11D	109.5
C5—C6—C1	120.6 (2)	H11C—C11A—H11D	108.1
S1—N1—C7—N2	173.72 (17)	C2—C1—C6—C5	-0.3 (3)
S1—N1—C7—C8	-5.4 (3)	C2—C3—C4—F8	-179.0 (2)
S1—C1—C2—C3	-178.33 (18)	C2—C3—C4—C5	1.0 (4)
S1—C1—C6—C5	178.44 (17)	O2—S1—N1—C7	-176.12 (19)
N2—C7—C8—C9	-59.1 (3)	O2—S1—C1—C2	75.1 (2)
N2—C7—C8—C12	67.2 (3)	O2—S1—C1—C6	-103.6 (2)
N2—C13—C14—O3	57.2 (3)	C13—N2—C7—N1	174.8 (2)
N2—C16—C15—O3	-57.1 (2)	C13—N2—C7—C8	-6.0 (3)
N1—S1—C1—C2	-37.6 (2)	C13—N2—C16—C15	54.2 (2)
N1—S1—C1—C6	143.67 (18)	C3—C4—C5—C6	-0.9 (4)
N1—C7—C8—C9	120.0 (2)	C4—C5—C6—C1	0.5 (4)
N1—C7—C8—C12	-113.8 (2)	C16—N2—C7—N1	-1.2 (3)

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C1—S1—N1—C7	-62.4 (2)	C16—N2—C7—C8	177.91 (19)
C1—C2—C3—C4	-0.7 (4)	C16—N2—C13—C14	-54.0 (2)
C7—N2—C13—C14	129.6 (2)	C14—O3—C15—C16	59.7 (2)
C7—N2—C16—C15	-129.2 (2)	C9—C8—C12—C11	-28.7 (3)
C7—C8—C9—C10	141.5 (2)	C9—C8—C12—C11A	0.3 (7)
C7—C8—C12—C11	-159.9 (3)	C9—C10—C11A—C12	20.5 (12)
C7—C8—C12—C11A	-130.8 (7)	C6—C1—C2—C3	0.4 (4)
O1—S1—N1—C7	55.6 (2)	C12—C8—C9—C10	10.5 (3)
O1—S1—C1—C2	-159.96 (18)	C12—C11—C10—C9	-30.9 (4)
O1—S1—C1—C6	21.3 (2)	C12—C11—C10—C11A	67.4 (15)
C8—C9—C10—C11	12.6 (4)	C15—O3—C14—C13	-59.8 (3)
C8—C9—C10—C11A	-19.4 (8)	C11—C12—C11A—C10	78.1 (15)
C8—C12—C11—C10	36.4 (4)	C11—C10—C11A—C12	-72.0 (15)
C8—C12—C11A—C10	-12.9 (12)	C11A—C12—C11—C10	-59.6 (15)
F8—C4—C5—C6	179.1 (2)		

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