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(*Z*)-4-Chloro-*N*-{3-[(4-chlorophenyl)sulfonyl]-2,3-dihydrobenzo[*d*]thiazol-2-ylidene}benzenesulfonamide

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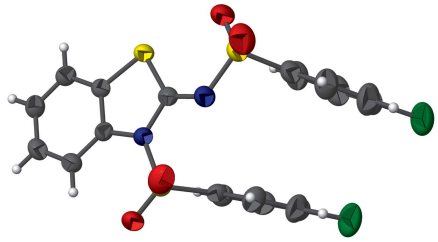
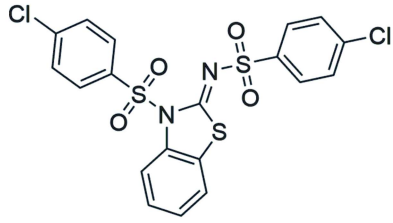
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{19}H_{12}Cl_2N_2O_4S_3$, is related to a ditosylated 2-imino-benzothiazole with the two methyl groups on the two phenyl rings replaced by chlorine. There is a weak intramolecular π–π contact between the two phenyl rings, with a centroid-to-centroid distance of 4.004 (2) Å. The dihedral angle between the rings is 9.96 (13)°. An intramolecular C—H···O hydrogen bond stabilizes the molecular conformation.

3D view



Chemical scheme



Structure description

The methylerythritolphosphate (MEP) pathway is an essential enzymatic pathway for the biosynthesis of isoprenoid precursors present in most bacteria, some protozoa and plants (Persch *et al.*, 2015; Frank & Groll, 2017; Hunter, 2007; Masini & Hirsch, 2014; Odom, 2011; Hale *et al.*, 2012). Inhibition of enzymes from this pathway has tremendous potential to generate new anti-infective agents or herbicides (Frank & Groll, 2017; Witschel *et al.*, 2013). The enzyme 2-methylerythritol 2,4-cyclodiphosphate synthase (IspF) is present in the MEP pathway (Zhang *et al.*, 2013, Geist *et al.*, 2010, Crane *et al.*, 2006). Recently, bis-sulfonamides of *ortho*-phenylenediamine have been shown to have micromolar inhibitory activity against IspF from *Arabidopsis thaliana*, *Plasmodium falciparum*, or *Burkholderia pseudomallei* (Thelemann *et al.*, 2015). In our quest to discover inhibitors of IspF, we synthesized a series of sulfonamide and bis-sulfonamide analogs of 2-aminobenzthiazole that would be capable of binding to the zinc ion of the IspF enzyme. This work resulted in the synthesis of the title compound.

The title compound, shown in Fig. 1, is closely related to a ditosylated 2-imino-benzothiazole (Castanheiro *et al.*, 2017) with the two methyl groups on the two phenyl groups replaced by chlorine. However, there are significant structural differences

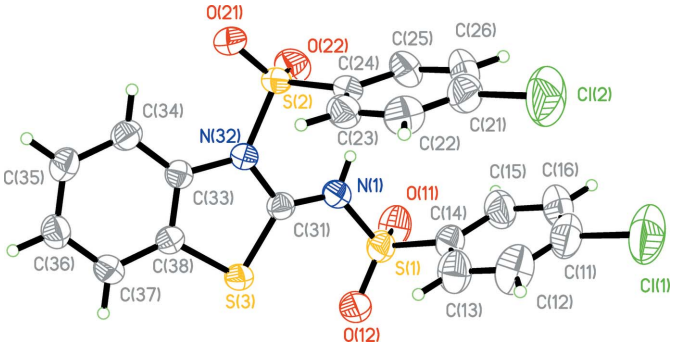


Figure 1
The molecular structure of the title compound, with displacement ellipsoids drawn at the 50% probability level.

between the structures of the two compounds. The title compound crystallizes in the space group $P\overline{1}$, whereas the methyl compound crystallizes in $P2_1/c$. Furthermore, the phenyl rings of the title compound lie on one side of the iminobenzothiazole plane, whereas they are on the other side in the methyl compound, as shown in Fig. 2. The torsion angles C31—N32—S2—C24 and C31—N1—S1—C14 in the title compound are −57.91 (16) and −122.8 (2)°, respectively. The corresponding torsion angles of the methyl compound are 60.9 (2) and 107.2 (2)°, respectively. Weak non-classical hydrogen bonds of the type C—H···O (Table 1) consolidate the molecular packing in the crystal (Fig. 3).

Synthesis and crystallization

2-Aminobenzothiazole (0.98 mmol) was dissolved in methylene chloride (5 ml) and pyridine (3.8 mmol) in an ice bath. 4-Chlorobenzenesulfonyl chloride (1.0 mmol) was added while stirring, and the reaction was allowed to come to room temperature. The reaction was monitored by TLC, and after 18 h the mixture was concentrated and the remaining solution in pyridine was extracted with water (100 ml) and ethyl acetate (80 ml). The organic layer was washed with brine (30 ml) and dried over anhydrous sodium sulfate. The combined extracts were concentrated to obtain the crude product, which was chromatographed (1: 2 *v*/*v* ethyl acetate/hexane) to yield the title compound (0.11 mmol, 11%). The material was recrystallized from a $CDCl_3$ solution.

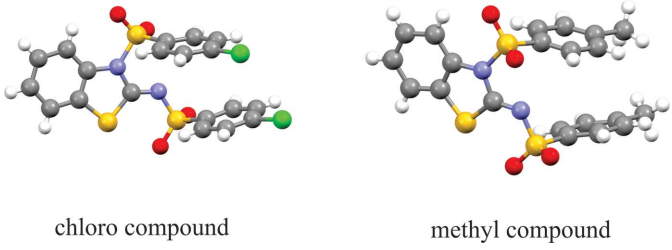


Figure 2
The molecular conformations of the title compound (left) and the methyl analog (right). The two phenyl groups of the title compound are above the plane of the iminobenzothiazole rings (the plane of the paper), while they are below the plane in the methyl analog.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12···O11^{i}	0.93	2.53	3.203 (3)	130
C22—H22···O22^{i}	0.93	2.59	3.249 (3)	128
C37—H37···O21^{ii}	0.93	2.50	3.339 (3)	151
C34—H34···O21	0.93	2.22	2.837 (3)	123

Symmetry codes: (i) $x-1, y, z$; (ii) $x, y-1, z$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{19}H_{12}Cl_2N_2O_4S_3$
M_r	499.39
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	293
a, b, c (Å)	7.1330 (9), 8.1155 (11), 17.798 (2)
α, β, γ (°)	87.747 (2), 81.840 (2), 87.849 (2)
V (Å^3)	1018.5 (2)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.66
Crystal size (mm)	0.60 × 0.30 × 0.25
Data collection	
Diffractometer	Bruker SMART CCD PLATFORM
Absorption correction	Multi-scan (*SADABS*; Bruker, 1999)
T_{min}, T_{max}	0.186, 0.264
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7549, 3530, 3301
R_{int}	0.016
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.036, 0.096, 1.04
No. of reflections	3530
No. of parameters	271
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.58, −0.62

Computer programs: *SMART* and *SAINT* (Bruker, 1999), *SIR97* (Altomare *et al.*, 1999), *SHELXL2016* (Sheldrick, 2015), *XP* in *SHELXTL* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2006) and *publCIF* (Westrip, 2010).

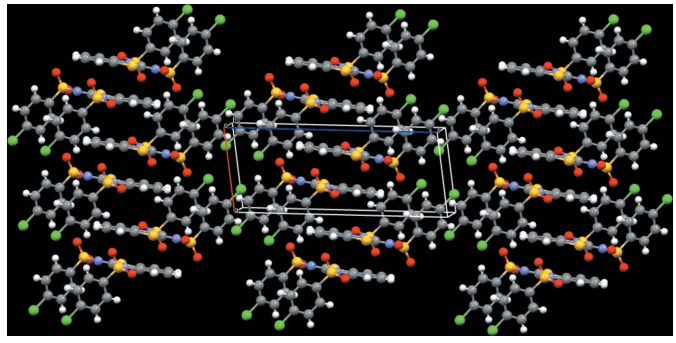


Figure 3
Packing of the title molecules viewed down the *b* axis. The white, grey, blue, red, yellow and green spheres are H, C, N, O, S and Cl atoms, respectively.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

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full crystallographic data

IUCrData (2017). **2**, x170865 [https://doi.org/10.1107/S2414314617008653]

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Crystal data

$C_{19}H_{12}Cl_2N_2O_4S_3$
M_r = 499.39
Triclinic, $P\overline{1}$
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b = 8.1155 (11) Å
c = 17.798 (2) Å
α = 87.747 (2)°
β = 81.840 (2)°
γ = 87.849 (2)°
V = 1018.5 (2) Å^3
Z = 2
$F(000)$ = 508
D_x = 1.628 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 906 reflections
θ = 2–14°
μ = 0.66 mm^{-1}
T = 293 K
Fragment, colorless
0.60 × 0.30 × 0.25 mm

Data collection

Bruker SMART CCD PLATFORM diffractometer
Radiation source: fine-focus sealed tube
Detector resolution: 0 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.186, T_{max} = 0.264
7549 measured reflections
3530 independent reflections
3301 reflections with $I > 2\sigma(I)$
R_{int} = 0.016
θ_{max} = 25.0°, θ_{min} = 2.3°
h = −8→8
k = −9→9
l = −21→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.096
S = 1.04
3530 reflections
271 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0448P)^2 + 0.6375P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.62 e Å^{-3}

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.37024 (8)	0.03706 (7)	0.77485 (3)	0.04724 (16)
S2	0.28022 (8)	0.43662 (6)	0.60143 (3)	0.04326 (16)
S3	0.29160 (7)	−0.08482 (6)	0.60835 (3)	0.03773 (15)
Cl1	−0.25853 (15)	0.26317 (14)	1.03311 (5)	0.1060 (4)
Cl2	−0.35272 (13)	0.55565 (14)	0.87265 (5)	0.1002 (3)
N1	0.3383 (3)	0.1643 (2)	0.70469 (10)	0.0446 (4)
C11	−0.0832 (4)	0.2042 (4)	0.95977 (15)	0.0698 (8)
O11	0.5492 (2)	0.0699 (3)	0.79694 (10)	0.0662 (5)
C12	−0.1312 (4)	0.1098 (4)	0.90386 (16)	0.0744 (8)
H12	−0.255949	0.079825	0.904470	0.089*
O12	0.3336 (3)	−0.1291 (2)	0.75832 (9)	0.0611 (5)
C13	0.0077 (4)	0.0596 (4)	0.84652 (15)	0.0634 (7)
H13	−0.022673	−0.004985	0.808228	0.076*
C14	0.1913 (3)	0.1057 (3)	0.84637 (12)	0.0486 (5)
C15	0.2376 (4)	0.2030 (4)	0.90258 (15)	0.0651 (7)
H15	0.361647	0.235004	0.901832	0.078*
C16	0.0982 (5)	0.2520 (4)	0.95971 (16)	0.0771 (8)
H16	0.127549	0.317278	0.997969	0.092*
C21	−0.1739 (4)	0.5178 (3)	0.79780 (14)	0.0581 (6)
O21	0.2169 (3)	0.52024 (18)	0.53771 (9)	0.0608 (5)
C22	−0.2195 (3)	0.4463 (3)	0.73429 (15)	0.0568 (6)
H22	−0.343084	0.416516	0.731865	0.068*
O22	0.4612 (2)	0.4680 (2)	0.62072 (10)	0.0604 (5)
C23	−0.0786 (3)	0.4197 (3)	0.67448 (13)	0.0481 (5)
H23	−0.106709	0.374468	0.630332	0.058*
C24	0.1050 (3)	0.4603 (2)	0.68022 (11)	0.0390 (4)
C25	0.1500 (3)	0.5307 (3)	0.74424 (14)	0.0527 (6)
H25	0.274276	0.557063	0.747588	0.063*
C26	0.0074 (4)	0.5613 (3)	0.80321 (14)	0.0634 (7)
H26	0.033945	0.611211	0.846482	0.076*
C31	0.3056 (3)	0.1145 (2)	0.63973 (11)	0.0364 (4)
N32	0.2750 (2)	0.23124 (19)	0.58320 (9)	0.0380 (4)
C33	0.2499 (3)	0.1635 (2)	0.51252 (11)	0.0341 (4)
C34	0.2275 (3)	0.2439 (3)	0.44425 (12)	0.0421 (5)
H34	0.223853	0.358527	0.439781	0.051*
C35	0.2108 (3)	0.1491 (3)	0.38283 (12)	0.0444 (5)
H35	0.194170	0.201233	0.336651	0.053*
C36	0.2181 (3)	−0.0213 (3)	0.38840 (12)	0.0446 (5)
H36	0.207626	−0.081849	0.346003	0.054*
C37	0.2409 (3)	−0.1021 (3)	0.45611 (12)	0.0408 (4)
H37	0.245905	−0.216761	0.460103	0.049*
C38	0.2561 (3)	−0.0077 (2)	0.51843 (11)	0.0344 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0575 (3)	0.0479 (3)	0.0374 (3)	0.0024 (2)	−0.0118 (2)	−0.0003 (2)
S2	0.0554 (3)	0.0303 (3)	0.0419 (3)	−0.0057 (2)	0.0020 (2)	−0.0013 (2)
S3	0.0444 (3)	0.0310 (3)	0.0382 (3)	−0.00082 (19)	−0.0080 (2)	0.00066 (19)
Cl1	0.1077 (7)	0.1351 (8)	0.0629 (5)	0.0373 (6)	0.0185 (4)	0.0011 (5)
Cl2	0.0861 (6)	0.1271 (8)	0.0752 (5)	0.0237 (5)	0.0257 (4)	−0.0123 (5)
N1	0.0580 (11)	0.0396 (9)	0.0371 (9)	−0.0001 (8)	−0.0102 (8)	−0.0020 (7)
C11	0.0794 (19)	0.0823 (19)	0.0431 (14)	0.0196 (15)	0.0004 (13)	0.0029 (13)
O11	0.0552 (10)	0.0930 (14)	0.0529 (10)	0.0019 (9)	−0.0177 (8)	−0.0013 (9)
C12	0.0550 (15)	0.106 (2)	0.0613 (17)	0.0027 (15)	−0.0084 (13)	0.0035 (16)
O12	0.0945 (13)	0.0420 (9)	0.0471 (9)	0.0052 (8)	−0.0141 (9)	0.0016 (7)
C13	0.0618 (16)	0.0836 (19)	0.0475 (13)	−0.0034 (13)	−0.0154 (12)	−0.0072 (12)
C14	0.0582 (13)	0.0509 (13)	0.0373 (11)	−0.0007 (10)	−0.0100 (10)	0.0009 (9)
C15	0.0734 (17)	0.0726 (17)	0.0507 (14)	−0.0130 (14)	−0.0076 (12)	−0.0140 (12)
C16	0.097 (2)	0.084 (2)	0.0501 (15)	−0.0054 (17)	−0.0037 (15)	−0.0209 (14)
C21	0.0602 (15)	0.0570 (14)	0.0524 (14)	0.0115 (11)	0.0045 (11)	−0.0013 (11)
O21	0.1006 (14)	0.0339 (8)	0.0444 (9)	0.0050 (8)	−0.0013 (8)	0.0044 (7)
C22	0.0466 (13)	0.0589 (14)	0.0638 (15)	0.0001 (11)	−0.0053 (11)	0.0003 (12)
O22	0.0537 (10)	0.0565 (10)	0.0687 (11)	−0.0206 (8)	0.0060 (8)	−0.0099 (8)
C23	0.0537 (13)	0.0443 (12)	0.0478 (12)	−0.0029 (10)	−0.0115 (10)	−0.0051 (9)
C24	0.0473 (11)	0.0286 (9)	0.0405 (11)	−0.0001 (8)	−0.0041 (9)	−0.0028 (8)
C25	0.0536 (13)	0.0529 (13)	0.0537 (13)	−0.0041 (10)	−0.0096 (10)	−0.0158 (11)
C26	0.0749 (18)	0.0683 (16)	0.0480 (14)	0.0060 (13)	−0.0088 (12)	−0.0228 (12)
C31	0.0372 (10)	0.0342 (10)	0.0371 (10)	0.0003 (8)	−0.0032 (8)	0.0004 (8)
N32	0.0482 (9)	0.0302 (8)	0.0349 (8)	0.0010 (7)	−0.0039 (7)	−0.0014 (6)
C33	0.0310 (9)	0.0351 (10)	0.0352 (10)	0.0003 (7)	−0.0014 (7)	−0.0028 (8)
C34	0.0455 (11)	0.0394 (11)	0.0405 (11)	0.0004 (9)	−0.0046 (9)	0.0032 (9)
C35	0.0461 (11)	0.0517 (12)	0.0360 (11)	−0.0025 (9)	−0.0092 (9)	0.0039 (9)
C36	0.0457 (11)	0.0500 (12)	0.0393 (11)	−0.0057 (9)	−0.0077 (9)	−0.0063 (9)
C37	0.0420 (11)	0.0370 (10)	0.0441 (11)	−0.0045 (8)	−0.0067 (9)	−0.0049 (9)
C38	0.0303 (9)	0.0357 (10)	0.0367 (10)	−0.0017 (7)	−0.0033 (7)	0.0008 (8)

Geometric parameters (Å, º)

S1—O11	1.4252 (18)	C21—C26	1.370 (4)
S1—O12	1.4331 (18)	C21—C22	1.375 (4)
S1—N1	1.6244 (18)	C22—C23	1.374 (3)
S1—C14	1.761 (2)	C22—H22	0.9300
S2—O22	1.4165 (18)	C23—C24	1.381 (3)
S2—O21	1.4186 (17)	C23—H23	0.9300
S2—N32	1.7133 (16)	C24—C25	1.377 (3)
S2—C24	1.752 (2)	C25—C26	1.377 (3)
S3—C31	1.743 (2)	C25—H25	0.9300
S3—C38	1.7439 (19)	C26—H26	0.9300
Cl1—C11	1.743 (3)	C31—N32	1.389 (3)
Cl2—C21	1.737 (2)	N32—C33	1.429 (2)

N1—C31	1.294 (3)	C33—C34	1.383 (3)
C11—C16	1.365 (4)	C33—C38	1.389 (3)
C11—C12	1.368 (4)	C34—C35	1.383 (3)
C12—C13	1.380 (4)	C34—H34	0.9300
C12—H12	0.9300	C35—C36	1.382 (3)
C13—C14	1.375 (3)	C35—H35	0.9300
C13—H13	0.9300	C36—C37	1.376 (3)
C14—C15	1.381 (3)	C36—H36	0.9300
C15—C16	1.377 (4)	C37—C38	1.391 (3)
C15—H15	0.9300	C37—H37	0.9300
C16—H16	0.9300		

O11—S1—O12	118.29 (12)	C21—C22—H22	120.7
O11—S1—N1	107.50 (11)	C22—C23—C24	119.7 (2)
O12—S1—N1	111.51 (9)	C22—C23—H23	120.2
O11—S1—C14	108.24 (11)	C24—C23—H23	120.2
O12—S1—C14	108.49 (11)	C25—C24—C23	121.4 (2)
N1—S1—C14	101.45 (10)	C25—C24—S2	119.38 (17)
O22—S2—O21	119.94 (11)	C23—C24—S2	119.02 (16)
O22—S2—N32	108.05 (10)	C26—C25—C24	118.7 (2)
O21—S2—N32	104.94 (9)	C26—C25—H25	120.7
O22—S2—C24	110.58 (10)	C24—C25—H25	120.7
O21—S2—C24	108.54 (10)	C21—C26—C25	119.7 (2)
N32—S2—C24	103.39 (9)	C21—C26—H26	120.2
C31—S3—C38	90.95 (9)	C25—C26—H26	120.2
C31—N1—S1	122.39 (15)	N1—C31—N32	118.90 (18)
C16—C11—C12	121.6 (3)	N1—C31—S3	130.18 (16)
C16—C11—Cl1	119.4 (2)	N32—C31—S3	110.92 (14)
C12—C11—Cl1	118.9 (3)	C31—N32—C33	114.44 (16)
C11—C12—C13	119.2 (3)	C31—N32—S2	119.26 (13)
C11—C12—H12	120.4	C33—N32—S2	126.24 (13)
C13—C12—H12	120.4	C34—C33—C38	120.44 (18)
C14—C13—C12	119.6 (3)	C34—C33—N32	129.24 (18)
C14—C13—H13	120.2	C38—C33—N32	110.29 (16)
C12—C13—H13	120.2	C35—C34—C33	118.10 (19)
C13—C14—C15	120.7 (2)	C35—C34—H34	120.9
C13—C14—S1	119.75 (18)	C33—C34—H34	120.9
C15—C14—S1	119.6 (2)	C36—C35—C34	121.6 (2)
C16—C15—C14	119.4 (3)	C36—C35—H35	119.2
C16—C15—H15	120.3	C34—C35—H35	119.2
C14—C15—H15	120.3	C37—C36—C35	120.63 (19)
C11—C16—C15	119.5 (3)	C37—C36—H36	119.7
C11—C16—H16	120.2	C35—C36—H36	119.7
C15—C16—H16	120.2	C36—C37—C38	118.20 (19)
C26—C21—C22	121.9 (2)	C36—C37—H37	120.9
C26—C21—Cl2	119.4 (2)	C38—C37—H37	120.9
C22—C21—Cl2	118.7 (2)	C33—C38—C37	121.04 (18)
C23—C22—C21	118.6 (2)	C33—C38—S3	113.31 (14)

C23—C22—H22	120.7	C37—C38—S3	125.62 (15)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12···O11^{i}	0.93	2.53	3.203 (3)	130
C22—H22···O22^{i}	0.93	2.59	3.249 (3)	128
C37—H37···O21^{ii}	0.93	2.50	3.339 (3)	151
C34—H34···O21	0.93	2.22	2.837 (3)	123

Symmetry codes: (i) $x-1, y, z$; (ii) $x, y-1, z$.