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1-((*E*)-{2-[4-(2-{(1*E*)-[(carbamothioylamino)imino]methyl}phenoxy)butoxy]benzylidene}amino)thiourea dimethyl sulfoxide disolvate

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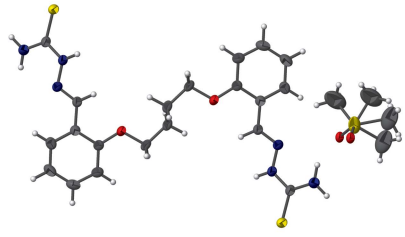
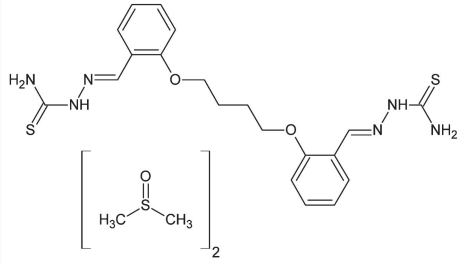
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{20}H_{24}N_6O_2S_2\cdot 2C_2H_6OS$, has crystallographically imposed centrosymmetry. The packing is assisted by N—H···O, C—H···O and N—H···S interactions with the lattice solvent molecules, forming a two-dimensional network parallel to (110). The lattice dimethyl sulfoxide molecules (except for the S atoms) were modelled over two sites with refined occupancies of 0.831 (3):0.169 (3).

3D view



Chemical scheme



Structure description

Thiosemicarbazones and their metal complexes have been known and interest to chemists for over fifty years due to their wide spectrum of biological activity such as antitumor, antibiotic and antiviral properties (Adelstein, 1973; Pandeya & Dimmock, 1993; Quiroga, *et al.*, 1998; Christlieb & Dilworth, 2006). The synthesis of bis functionalized compounds are considered as significant precursors for building blocks of vital molecules such as nanoscience and supramolecular chemistry (Holland *et al.*, 2007), and binucleating ligand designs (Gavrilova & Bosnich, 2004). In this context we report in this study the synthesis and crystal structure of the title compound.

The title molecule (Fig. 1) has crystallographically imposed centrosymmetry. In the crystal, the packing is assisted by N—H···O, C—H···O and N—H···S interactions with the lattice DMSO molecules (Table 1 and Fig. 2), forming a two-dimensional network parallel to (110)

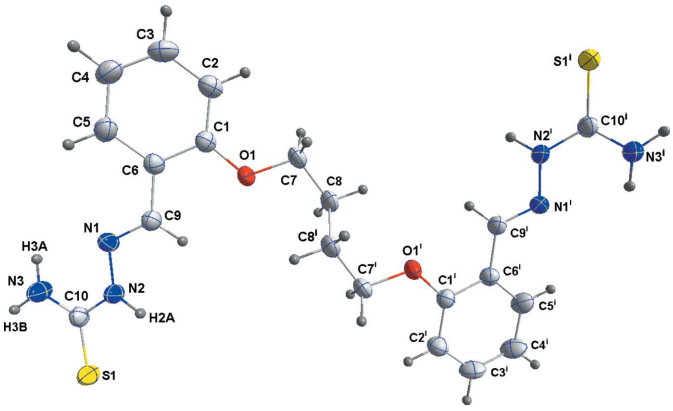


Figure 1
The title molecule, showing the atom-labeling scheme and 50% probability displacement ellipsoids [symmetry code: (i) $-x, -y, 1-z$].

Synthesis and crystallization

Salicyldehyde 122 mg (1 mmol) in hot ethanolic potassium hydroxide solution (prepared by dissolving 56 mg (1 mmol) of KOH in 10 ml of absolute ethanol) was stirred until a clear solution was obtained. The solution was evaporated under vacuum and the residue was dissolved in 5 ml DMF and then 119.4 µl (0.5 mmol) of 1,4-dibromobutane was added. The reaction mixture was refluxed for 5 minutes. The resulted potassium bromide was separated by filtration and the filtrate was then evaporated under *vacuum*. The remaining solid was washed with water and crystallized from ethanol to give high quality crystals (m.p. 513 K) suitable for X-ray analysis in a good yield (90%).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The lattice DMSO molecules (except S atoms) were modelled over two sites with refined occupancies of 0.831 (3):0.169 (3).

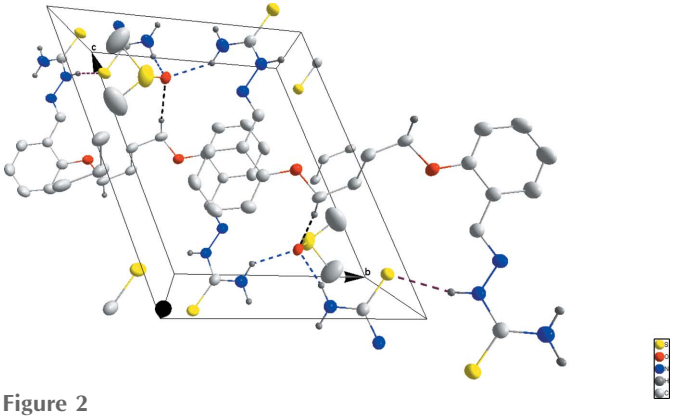


Figure 2
Packing viewed down the *a* axis. Intermolecular N—H···O, C—H···O and N—H···S hydrogen bonds are shown, respectively, as blue, black and purple dotted lines.

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···S1^{i}	0.91	2.49	3.371 (2)	163
N3—H3A···O2	0.91	2.14	2.887 (3)	139
N3—H3B···O2^{ii}	0.91	2.04	2.885 (3)	153
C7—H7B···O2^{iii}	0.99	2.49	3.471 (3)	174

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{20}H_{24}N_6O_2S_2{\cdot}2C_2H_6OS$
M_r	600.83
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	150
a, b, c (Å)	7.2571 (2), 9.7909 (2), 12.0060 (2)
α, β, γ (°)	112.984 (1), 98.163 (1), 96.909 (1)
V (Å^3)	762.80 (3)
Z	1
Radiation type	Cu $K\alpha$
μ (mm^{-1})	3.19
Crystal size (mm)	0.24 × 0.15 × 0.09
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2015)
T_{min}, T_{max}	0.65, 0.76
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8374, 2932, 2679
R_{int}	0.023
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.056, 0.162, 1.08
No. of reflections	2932
No. of parameters	183
No. of restraints	27
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.88, −0.68

Computer programs: *APEX2* and *SAINT* (Bruker, 2015), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

Acknowledgements

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full crystallographic data

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1-((*E*)-{2-[4-(2-{(1*E*)-[(carbamothioylamino)imino]methyl}phenoxy)butoxy]-benzylidene}amino)thiourea dimethyl sulfoxide disolvate

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1-((*E*)-{2-[4-(2-{(1*E*)-[(Carbamothioylamino)imino]methyl}phenoxy)butoxy]benzylidene}amino)thiourea dimethyl sulfoxide disolvate

Crystal data

$C_{20}H_{24}N_6O_2S_2\cdot 2C_2H_6OS$
M_r = 600.83
Triclinic, $P\overline{1}$
a = 7.2571 (2) Å
b = 9.7909 (2) Å
c = 12.0060 (2) Å
α = 112.984 (1)°
β = 98.163 (1)°
γ = 96.909 (1)°
V = 762.80 (3) Å^3
Z = 1
$F(000)$ = 318
D_x = 1.308 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 6799 reflections
θ = 4.1–72.1°
μ = 3.19 mm^{-1}
T = 150 K
Thick plate, colourless
0.24 × 0.15 × 0.09 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC IμS micro–focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2015)
T_{min} = 0.65, T_{max} = 0.76
8374 measured reflections
2932 independent reflections
2679 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 72.1°, θ_{min} = 5.0°
h = −8→8
k = −12→11
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.162
S = 1.08
2932 reflections
183 parameters
27 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0905P)^2 + 0.766P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.88 e Å^{-3}
$\Delta\rho_{min}$ = −0.68 e Å^{-3}
Extinction correction: SHELXL2014 (Sheldrick, 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0061 (13)

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.

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 $F^2 > 2\text{sigma}(F^2)$ 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. H-atoms attached to carbon were placed in calculated positions (C—H = 0.95 - 0.99 Å) while those attached to nitrogen were placed in locations derived from a difference map and their parameters adjusted to give N—H = 0.91 Å. All were included as riding contributions with isotropic displacement parameters 1.2 times those of the attached atoms.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
S1	0.18022 (10)	0.04286 (7)	−0.12107 (6)	0.0368 (2)	
O1	0.1735 (3)	0.2497 (2)	0.51184 (15)	0.0357 (4)	
N1	0.2228 (3)	0.3358 (2)	0.22135 (18)	0.0304 (5)	
N2	0.1727 (3)	0.2071 (2)	0.11133 (19)	0.0332 (5)	
H2A	0.0875	0.1248	0.1011	0.040*	
N3	0.3466 (3)	0.3281 (3)	0.0209 (2)	0.0390 (5)	
H3A	0.3769	0.4102	0.0950	0.047*	
H3B	0.3708	0.3273	−0.0516	0.047*	
C1	0.2179 (3)	0.4002 (3)	0.5403 (2)	0.0300 (5)	
C2	0.2562 (4)	0.5137 (3)	0.6594 (2)	0.0370 (6)	
H2	0.2490	0.4888	0.7279	0.044*	
C3	0.3048 (4)	0.6632 (3)	0.6779 (3)	0.0411 (7)	
H3	0.3303	0.7408	0.7593	0.049*	
C4	0.3165 (4)	0.7009 (3)	0.5790 (3)	0.0431 (7)	
H4	0.3500	0.8038	0.5926	0.052*	
C5	0.2792 (4)	0.5879 (3)	0.4600 (3)	0.0378 (6)	
H5	0.2889	0.6139	0.3923	0.045*	
C6	0.2279 (3)	0.4369 (3)	0.4385 (2)	0.0284 (5)	
C7	0.1356 (4)	0.2043 (3)	0.6080 (2)	0.0372 (6)	
H7A	0.0272	0.2458	0.6410	0.045*	
H7B	0.2480	0.2418	0.6766	0.045*	
C8	0.0894 (4)	0.0336 (3)	0.5507 (2)	0.0383 (6)	
H8A	0.0738	−0.0015	0.6164	0.046*	
H8B	0.1978	−0.0051	0.5157	0.046*	
C9	0.1840 (3)	0.3150 (3)	0.3144 (2)	0.0297 (5)	
H9	0.1248	0.2170	0.3027	0.036*	
C10	0.2385 (4)	0.2042 (3)	0.0115 (2)	0.0301 (5)	
S2	0.29091 (12)	0.73336 (10)	0.18388 (10)	0.0576 (3)	
O2	0.4525 (3)	0.6510 (2)	0.16444 (18)	0.0268 (5)	0.831 (3)
C11	0.3689 (11)	0.9102 (8)	0.2855 (8)	0.114 (2)	0.831 (3)
H11A	0.2621	0.9631	0.2976	0.172*	0.831 (3)
H11B	0.4297	0.9117	0.3644	0.172*	0.831 (3)
H11C	0.4612	0.9606	0.2549	0.172*	0.831 (3)

C12	0.2625 (10)	0.7934 (10)	0.0557 (7)	0.101 (2)	0.831 (3)
H12A	0.1582	0.8491	0.0607	0.151*	0.831 (3)
H12B	0.3802	0.8588	0.0617	0.151*	0.831 (3)
H12C	0.2338	0.7041	−0.0233	0.151*	0.831 (3)
O2A	0.0956 (8)	0.6372 (9)	0.1245 (8)	0.0268 (5)	0.169 (3)
C11A	0.207 (5)	0.760 (4)	0.310 (2)	0.114 (2)	0.169 (3)
H11D	0.3039	0.8269	0.3829	0.172*	0.169 (3)
H11E	0.0943	0.8055	0.3075	0.172*	0.169 (3)
H11F	0.1722	0.6622	0.3142	0.172*	0.169 (3)
C12A	0.334 (5)	0.907 (3)	0.158 (4)	0.101 (2)	0.169 (3)
H12D	0.4631	0.9624	0.1997	0.151*	0.169 (3)
H12E	0.3171	0.8803	0.0693	0.151*	0.169 (3)
H12F	0.2430	0.9705	0.1919	0.151*	0.169 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0455 (4)	0.0330 (4)	0.0280 (4)	−0.0013 (3)	0.0110 (3)	0.0099 (3)
O1	0.0514 (11)	0.0308 (9)	0.0257 (8)	0.0010 (8)	0.0113 (8)	0.0135 (7)
N1	0.0320 (11)	0.0314 (10)	0.0261 (10)	0.0012 (8)	0.0052 (8)	0.0117 (8)
N2	0.0401 (12)	0.0296 (10)	0.0274 (10)	−0.0034 (9)	0.0081 (9)	0.0118 (9)
N3	0.0461 (13)	0.0339 (11)	0.0339 (11)	−0.0024 (10)	0.0159 (10)	0.0111 (9)
C1	0.0280 (12)	0.0319 (12)	0.0297 (12)	0.0047 (10)	0.0065 (9)	0.0126 (10)
C2	0.0378 (14)	0.0398 (14)	0.0296 (13)	0.0060 (11)	0.0068 (10)	0.0110 (11)
C3	0.0386 (14)	0.0357 (14)	0.0353 (14)	0.0084 (11)	0.0011 (11)	0.0025 (11)
C4	0.0475 (16)	0.0275 (13)	0.0458 (16)	0.0069 (12)	−0.0012 (13)	0.0101 (12)
C5	0.0405 (15)	0.0322 (13)	0.0400 (14)	0.0051 (11)	0.0002 (11)	0.0176 (11)
C6	0.0266 (12)	0.0299 (12)	0.0288 (12)	0.0056 (9)	0.0046 (9)	0.0127 (10)
C7	0.0448 (15)	0.0438 (15)	0.0241 (12)	0.0005 (12)	0.0049 (10)	0.0184 (11)
C8	0.0464 (16)	0.0416 (14)	0.0301 (13)	0.0015 (12)	0.0018 (12)	0.0223 (12)
C9	0.0306 (12)	0.0293 (12)	0.0292 (12)	0.0025 (10)	0.0052 (9)	0.0134 (10)
C10	0.0306 (12)	0.0329 (12)	0.0293 (12)	0.0040 (10)	0.0071 (9)	0.0159 (10)
S2	0.0506 (5)	0.0574 (5)	0.0882 (7)	0.0202 (4)	0.0388 (4)	0.0433 (5)
O2	0.0279 (10)	0.0273 (10)	0.0312 (10)	0.0059 (8)	0.0099 (8)	0.0171 (8)
C11	0.109 (5)	0.077 (4)	0.140 (6)	0.023 (3)	0.055 (4)	0.014 (4)
C12	0.085 (4)	0.144 (5)	0.127 (5)	0.054 (4)	0.036 (4)	0.098 (4)
O2A	0.0279 (10)	0.0273 (10)	0.0312 (10)	0.0059 (8)	0.0099 (8)	0.0171 (8)
C11A	0.109 (5)	0.077 (4)	0.140 (6)	0.023 (3)	0.055 (4)	0.014 (4)
C12A	0.085 (4)	0.144 (5)	0.127 (5)	0.054 (4)	0.036 (4)	0.098 (4)

Geometric parameters (Å, º)

S1—C10	1.700 (3)	C7—H7B	0.9900
O1—C1	1.360 (3)	C8—C8^{i}	1.523 (5)
O1—C7	1.438 (3)	C8—H8A	0.9900
N1—C9	1.274 (3)	C8—H8B	0.9900
N1—N2	1.385 (3)	C9—H9	0.9500
N2—C10	1.343 (3)	S2—O2	1.496 (2)

N2—H2A	0.9101	S2—O2A	1.508 (4)
N3—C10	1.319 (3)	S2—C11	1.651 (7)
N3—H3A	0.9100	S2—C11A	1.651 (8)
N3—H3B	0.9101	S2—C12A	1.841 (7)
C1—C2	1.389 (4)	S2—C12	1.844 (6)
C1—C6	1.411 (3)	C11—H11A	0.9800
C2—C3	1.385 (4)	C11—H11B	0.9800
C2—H2	0.9500	C11—H11C	0.9800
C3—C4	1.384 (4)	C12—H12A	0.9800
C3—H3	0.9500	C12—H12B	0.9800
C4—C5	1.387 (4)	C12—H12C	0.9800
C4—H4	0.9500	C11A—H11D	0.9800
C5—C6	1.390 (4)	C11A—H11E	0.9800
C5—H5	0.9500	C11A—H11F	0.9800
C6—C9	1.460 (3)	C12A—H12D	0.9800
C7—C8	1.510 (4)	C12A—H12E	0.9800
C7—H7A	0.9900	C12A—H12F	0.9800

C1—O1—C7	118.3 (2)	H8A—C8—H8B	107.7
C9—N1—N2	114.0 (2)	N1—C9—C6	122.0 (2)
C10—N2—N1	120.4 (2)	N1—C9—H9	119.0
C10—N2—H2A	117.1	C6—C9—H9	119.0
N1—N2—H2A	122.4	N3—C10—N2	118.0 (2)
C10—N3—H3A	119.0	N3—C10—S1	122.66 (19)
C10—N3—H3B	115.2	N2—C10—S1	119.34 (18)
H3A—N3—H3B	125.2	O2—S2—C11	110.1 (3)
O1—C1—C2	124.6 (2)	O2A—S2—C11A	81.0 (14)
O1—C1—C6	115.2 (2)	O2A—S2—C12A	114.8 (11)
C2—C1—C6	120.2 (2)	C11A—S2—C12A	112.6 (17)
C3—C2—C1	119.7 (3)	O2—S2—C12	103.4 (2)
C3—C2—H2	120.2	C11—S2—C12	91.0 (4)
C1—C2—H2	120.2	S2—C11—H11A	109.5
C4—C3—C2	120.7 (3)	S2—C11—H11B	109.5
C4—C3—H3	119.6	H11A—C11—H11B	109.5
C2—C3—H3	119.6	S2—C11—H11C	109.5
C3—C4—C5	119.8 (3)	H11A—C11—H11C	109.5
C3—C4—H4	120.1	H11B—C11—H11C	109.5
C5—C4—H4	120.1	S2—C12—H12A	109.5
C4—C5—C6	120.7 (3)	S2—C12—H12B	109.5
C4—C5—H5	119.6	H12A—C12—H12B	109.5
C6—C5—H5	119.6	S2—C12—H12C	109.5
C5—C6—C1	118.9 (2)	H12A—C12—H12C	109.5
C5—C6—C9	122.4 (2)	H12B—C12—H12C	109.5
C1—C6—C9	118.8 (2)	S2—C11A—H11D	109.5
O1—C7—C8	106.9 (2)	S2—C11A—H11E	109.5
O1—C7—H7A	110.3	H11D—C11A—H11E	109.5
C8—C7—H7A	110.3	S2—C11A—H11F	109.5
O1—C7—H7B	110.3	H11D—C11A—H11F	109.5

C8—C7—H7B	110.3	H11E—C11A—H11F	109.5
H7A—C7—H7B	108.6	S2—C12A—H12D	109.5
C7—C8—C8^{i}	113.8 (3)	S2—C12A—H12E	109.5
C7—C8—H8A	108.8	H12D—C12A—H12E	109.5
C8^{i}—C8—H8A	108.8	S2—C12A—H12F	109.5
C7—C8—H8B	108.8	H12D—C12A—H12F	109.5
C8^{i}—C8—H8B	108.8	H12E—C12A—H12F	109.5
C9—N1—N2—C10	−166.5 (2)	C2—C1—C6—C5	1.0 (4)
C7—O1—C1—C2	9.7 (4)	O1—C1—C6—C9	2.2 (3)
C7—O1—C1—C6	−171.7 (2)	C2—C1—C6—C9	−179.1 (2)
O1—C1—C2—C3	178.3 (2)	C1—O1—C7—C8	179.6 (2)
C6—C1—C2—C3	−0.2 (4)	O1—C7—C8—C8^{i}	−63.5 (4)
C1—C2—C3—C4	−0.3 (4)	N2—N1—C9—C6	179.4 (2)
C2—C3—C4—C5	0.0 (5)	C5—C6—C9—N1	13.0 (4)
C3—C4—C5—C6	0.8 (4)	C1—C6—C9—N1	−166.9 (2)
C4—C5—C6—C1	−1.3 (4)	N1—N2—C10—N3	−1.9 (4)
C4—C5—C6—C9	178.8 (2)	N1—N2—C10—S1	178.10 (18)
O1—C1—C6—C5	−177.7 (2)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···S1^{ii}	0.91	2.49	3.371 (2)	163
N3—H3*A*···O2	0.91	2.14	2.887 (3)	139
N3—H3*B*···O2^{iii}	0.91	2.04	2.885 (3)	153
C7—H7*B*···O2^{iv}	0.99	2.49	3.471 (3)	174

Symmetry codes: (ii) −*x*, −*y*, −*z*; (iii) −*x*+1, −*y*+1, −*z*; (iv) −*x*+1, −*y*+1, −*z*+1.