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Improving the compatibility of fullerene acceptors with fluorene-containing donor-polymers in organic photovoltaic devices

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SHELXL97-2 & Manual Editing

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Drs. A. Meetsma

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2. PROCESSING SUMMARY (JOURNAL OFFICE ONLY)

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3. TITLE AND AUTHOR LIST

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;
Improving the compatibility of Fullerene Acceptors with Fluorene-Containing
Donor-Polymers in Organic Photovoltaic Devices
;
_publ_section_title_footnote      .
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The loop structure below should contain the names and addresses of all
authors, in the required order of publication. Repeat as necessary.

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_publ_author_name
'Jan-Carlos Kuhlmann'
'de Bruyn, Paul'
'Ricardo K. M. Bouwer'
'Auke Meetsma'
'Paul W. M. Blom'
'Jan C. Hummelen'
```

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loop_
_publ_author_address
;
Stratingh Institute for Chemistry,
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9747 AG Groningen,
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Fax: +31 50 363 8751;
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E-mail: j.c.hummelen@rug.nl
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;
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University of Groningen,
Nijenborgh 4,
9747 AG Groningen,
The Netherlands.
;
;
Dutch Polymer Institute,
P.O. Box 902,
5600 AX Eindhoven,
The Netherlands
;
```

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4. TEXT

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Insert blank lines between paragraphs

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_publ_section_comment
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_publ_section_exptl_prep
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;
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;
The hydrogen atoms were generated by geometrical considerations, constrained to
idealized geometries, and allowed to ride on the carrier atom with an
isotropic displacement parameter related to the equivalent displacement
parameter of their carrier atoms, with  $U_{iso}(H) = 1.2 U_{eq}(C)$ 
or  $1.5 U_{eq}(methyl\ C)$ . The methyl-groups were refined as rigid groups,
which were allowed to rotate freely. Assigned values of bond distances:
secondary C---H2 = 0.99 Å, methyl C---H3 = 0.98 Å and aromatic C---H =
0.95 Å. N---H = 0.86 Å.
;
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Bruker, (2007). <i>SMART</i> (Version 5.632), <i>SAINT-Plus</i> (Version
7.46a) and <i>SADABS</i> (Version 2.10). Bruker AXS Inc., Madison, Wisconsin,
USA.
```

Burla, M. C., Caliendo, R., Camalli, M., Carrozzini, B., Cascarano, G. L., De
Caro, L., Giacovazzo, C., Polidori, G. & Spagna, R. (2005). <i>SIR2004</i>. An
improved tool for crystal structure determination and refinement. J. Appl.
Cryst. 38, 381-388.

Meetsma, A. (2009). Extended version of the program <i>PLUTO</i>. University of
Groningen, The Netherlands. (unpublished).

Sheldrick, G. M. (2008). <i>Acta Cryst.</i> A**64**, 112--122.

Spek, A. L. (2003). <i>J. Appl. Cryst.</i> **36**, 7--13.

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Fig. 1. Perspective <i>PLUTO</i> drawings of the molecule illustrating the
configuration and the adopted numbering scheme.

Fig. 2. Molecular packing viewed down unit cell axes.

Fig. 3. Perspective <i>ORTEP</i> drawing of the title compound. Displacement
ellipsoids for non-H atoms are represented at the 40% probability level. The
H-atoms have been omitted to improve clarity.

Fig. 4. Perspective <i>PLUTO</i> drawing showing N---H...O hydrogen bonds shown
as dashed lines.

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;
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;
;
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_chemical_melting_point        ?
_chemical_formula_moiety        'C38 H50 N2 O4 S'
# Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)3, (C6 N6 Cr 3-)2, 2(H2 O)'
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_chemical_formula_iupac         ?
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C C 0.0033 0.0016 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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# 6. CRYSTAL DATA

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_symmetry_Int_Tables_number     2

loop_
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  _symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z

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_cell_length_b                  12.033(3)
_cell_length_c                  14.111(4)
_cell_angle_alpha               83.464(4)
_cell_angle_beta                81.891(4)
_cell_angle_gamma               69.071(3)
_cell_volume                    1795.7(8)
_cell_formula_units_Z           2

_cell_measurement_temperature   293(1)
_cell_measurement_reflns_used   3703
_cell_measurement_theta_min     2.92
_cell_measurement_theta_max     25.45
_cell_special_details

;
The final unit cell was obtained from the xyz centroids of
3703 reflections after integration using the SAINTPLUS
software package (Bruker, 2007).

Reduced cell calculations did not indicate any higher metric lattice symmetry
and examination of the final atomic coordinates of the structure did not
yield extra symmetry elements (Spek, 1988; Le Page 1987, 1988)
;

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_exptl_crystal_colour           colorless
_exptl_crystal_size_max         0.54

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_diffn_radiation_detector
;
CCD area-detector
;
_diffn_measurement_device_type
;
Bruker Smart Apex; CCD area detector
;
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;
Crystal into the cold nitrogen stream of the low-temperature unit
(KRYOFLEX, (Bruker, 2007)).
;
_diffn_detector_area_resol_mean 66.06

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_diffn_standard_refl_index_l
? ? ?

# number of measured reflections (redundant set)
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_diffn_reflns_av_sigmaI/netI    0.0362
_diffn_reflns_limit_h_min       -13
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_diffn_reflns_limit_k_max       14
_diffn_reflns_limit_l_min       -16
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_diffn_reflns_theta_full        25.00

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_diffrn_measured_fraction_theta_full 0.981

_diffrn_reflms_reduction_process
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Intensity data were corrected for Lorentz and polarization
effects, decay and absorption and reduced to  $F_o^2$ 
using SAINT-Plus & SADABS (Bruker, 2007).
;

# number of unique reflections
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_reflms_number_gt        4195
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_computing_cell_refinement 'SAINT-Plus (Bruker, 2007)'
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_computing_structure_solution
;
SIR2004 (Burla et al., 2005)
;
_computing_structure_refinement 'SHELXL-97 (Sheldrick, 2008)'
_computing_molecular_graphics
;
PLATON (Spek, 2003)
PLUTO (Meetsma, 2009)
;
_computing_publication_material 'PLATON (Spek, 2003)'

#####

# 8. REFINEMENT DATA

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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.
;

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_refine_ls_weighting_details
'calc w=1/[\sigma^2(Fo^2)+(0.0965P)^2+0.1255P] where P=(Fo^2+2Fc^2)/3'
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_atom_sites_solution_secondary direct
_atom_sites_solution_hydrogens geom
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_refine_ls_extinction_method none
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_refine_ls_abs_structure_details ?
_chemical_absolute_configuration .

_refine_ls_abs_structure_Flack ?
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_refine_ls_number_parameters  410
_refine_ls_number_restraints  0
_refine_ls_number_constraints ?
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_refine_ls_R_factor_gt        0.0563
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9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

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_atom_site_refinement_flags
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O2 O Uani -0.12615(16) 0.38629(15) -0.00930(13) 1.000 0.0731(7) . .
O3 O Uani 0.10264(19) -0.00286(16) -0.17363(14) 1.000 0.0886(8) . .
O4 O Uani 0.17579(19) -0.18417(15) -0.22674(13) 1.000 0.0814(7) . .
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C8 C Uani 0.1882(2) 0.0959(2) 0.06669(16) 1.000 0.0524(8) . .
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C14 C Uani 0.2673(2) 0.10373(19) 0.13876(15) 1.000 0.0502(7) . .
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C17 C Uani 0.4163(2) 0.1085(2) 0.27819(16) 1.000 0.0514(7) . .
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C24 C Uani 0.4372(3) 0.2945(3) 0.4566(2) 1.000 0.0820(11) . .
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 H34' H Uiso 0.14018 0.17718 0.40793 1.000 0.0813 . .
 H35 H Uiso 0.00729 0.34097 0.54731 1.000 0.0860 . .
 H35' H Uiso -0.05389 0.31969 0.46196 1.000 0.0860 . .
 H36 H Uiso 0.02892 0.15109 0.61520 1.000 0.0887 . .
 H36' H Uiso -0.02486 0.12414 0.52774 1.000 0.0887 . .
 H37 H Uiso -0.16738 0.29832 0.65773 1.000 0.1052 . .
 H37' H Uiso -0.22091 0.26973 0.57099 1.000 0.1052 . .
 H38 H Uiso -0.19706 0.07994 0.64387 1.000 0.1457 . .
 H38' H Uiso -0.28828 0.17987 0.70867 1.000 0.1457 . .
 H38'' H Uiso -0.14953 0.11303 0.73192 1.000 0.1457 . .

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O1 0.0719(12) 0.0713(11) 0.0984(13) -0.0092(10) -0.0408(10) -0.0227(9)
O2 0.0618(11) 0.0662(11) 0.0849(12) -0.0199(9) -0.0079(9) -0.0100(9)
O3 0.0982(15) 0.0633(12) 0.0980(14) -0.0280(10) -0.0390(12) -0.0030(11)
O4 0.0981(14) 0.0630(11) 0.0852(12) -0.0222(10) -0.0250(11) -0.0198(10)
N1 0.0623(12) 0.0515(11) 0.0750(12) -0.0067(10) -0.0282(10) -0.0176(10)
N2 0.0532(11) 0.0533(11) 0.0587(11) -0.0085(9) -0.0162(9) -0.0176(9)
C1 0.0619(15) 0.0528(14) 0.0604(14) -0.0094(11) -0.0244(12) -0.0104(12)
C2 0.094(2) 0.0732(18) 0.0847(19) -0.0325(16) -0.0072(17) -0.0315(17)
C3 0.099(2) 0.094(2) 0.0764(18) -0.0325(17) 0.0017(18) -0.0368(19)
C4 0.0767(18) 0.0750(18) 0.0613(15) -0.0020(14) -0.0188(14) -0.0228(15)
C5 0.089(2) 0.0544(14) 0.0630(15) -0.0049(13) -0.0174(15) -0.0199(14)
C6 0.0721(17) 0.0537(14) 0.0584(14) -0.0103(12) -0.0150(13) -0.0122(13)
C7 0.107(2) 0.103(2) 0.0700(18) 0.0019(17) -0.0098(18) -0.036(2)
C8 0.0524(13) 0.0488(13) 0.0559(13) -0.0053(10) -0.0075(11) -0.0163(11)
C9 0.0579(15) 0.0578(14) 0.0658(14) -0.0031(12) -0.0130(12) -0.0204(12)
C10 0.0582(16) 0.0738(17) 0.0795(17) -0.0132(14) -0.0109(14) -0.0185(13)
C11 0.0715(18) 0.0660(16) 0.0830(18) -0.0251(14) -0.0122(15) -0.0080(14)
C12 0.0725(17) 0.0569(15) 0.0676(15) -0.0161(13) -0.0073(14) -0.0168(14)
C13 0.124(3) 0.089(2) 0.097(2) -0.0211(18) -0.048(2) -0.028(2)
C14 0.0515(13) 0.0506(12) 0.0502(12) -0.0017(10) -0.0080(10) -0.0193(11)
C15 0.0575(14) 0.0474(13) 0.0656(14) -0.0079(11) -0.0104(12) -0.0126(11)
C16 0.0534(14) 0.0500(13) 0.0711(15) 0.0007(12) -0.0170(12) -0.0094(11)
C17 0.0464(12) 0.0539(13) 0.0549(12) 0.0023(10) -0.0092(10) -0.0192(11)
C18 0.0459(12) 0.0495(12) 0.0525(12) -0.0021(10) -0.0062(10) -0.0176(10)
C19 0.0461(12) 0.0483(12) 0.0539(12) -0.0022(10) -0.0106(10) -0.0138(10)
C20 0.0536(14) 0.0674(16) 0.0591(14) 0.0016(12) -0.0144(12) -0.0263(12)
C21 0.0658(17) 0.0847(19) 0.0812(18) 0.0015(15) -0.0283(15) -0.0211(15)
C22 0.080(2) 0.109(3) 0.096(2) -0.0018(19) -0.0464(18) -0.0274(19)
C23 0.093(2) 0.131(3) 0.088(2) -0.016(2) -0.0409(19) -0.045(2)
C24 0.0724(18) 0.098(2) 0.0816(18) -0.0236(16) -0.0175(15) -0.0283(16)
C25 0.0554(14) 0.0709(16) 0.0583(14) -0.0063(12) -0.0124(12) -0.0275(13)
C26 0.0508(13) 0.0558(13) 0.0608(13) -0.0106(11) -0.0082(11) -0.0181(11)
C27 0.0594(15) 0.0573(14) 0.0794(16) -0.0148(13) -0.0076(13) -0.0198(12)
C28 0.0614(16) 0.0575(15) 0.0836(17) -0.0021(13) -0.0088(14) -0.0215(12)
C29 0.074(2) 0.0640(18) 0.142(3) 0.0144(18) -0.014(2) -0.0230(16)
C30 0.087(2) 0.096(2) 0.100(2) 0.0321(18) -0.0351(18) -0.0528(18)
C31 0.117(3) 0.116(3) 0.239(5) 0.080(3) -0.027(4) -0.062(3)
C32 0.114(3) 0.131(3) 0.206(5) 0.073(3) -0.056(3) -0.064(3)
C33 0.0570(15) 0.0696(16) 0.0651(14) -0.0164(13) -0.0050(12) -0.0200(13)
C34 0.0608(16) 0.0776(18) 0.0658(15) -0.0118(13) -0.0036(13) -0.0245(14)
C35 0.0599(16) 0.0905(19) 0.0652(15) -0.0130(14) -0.0050(13) -0.0253(14)
C36 0.0743(18) 0.0874(19) 0.0658(15) -0.0119(15) -0.0038(14) -0.0346(16)
C37 0.076(2) 0.100(2) 0.0853(19) -0.0028(17) -0.0006(16) -0.0326(18)
C38 0.094(2) 0.122(3) 0.084(2) 0.0011(19) -0.0012(18) -0.054(2)

#=====

10. MOLECULAR GEOMETRY

_geom_special_details

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Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

;

loop_

_geom_bond_atom_site_label_1

_geom_bond_atom_site_label_2

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_geom_bond_site_symmetry_1

_geom_bond_site_symmetry_2

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S1 O2 1.4211(19) . . yes
S1 N1 1.644(2) . . yes
S1 C1 1.759(3) . . yes
O3 C12 1.203(3) . . yes
O4 C12 1.330(3) . . yes
O4 C13 1.437(4) . . yes
N1 N2 1.400(3) . . yes
N2 C8 1.283(3) . . yes
N1 H1 0.8600 . . no
C1 C2 1.383(4) . . no
C1 C6 1.382(3) . . no
C2 C3 1.367(5) . . no
C3 C4 1.398(5) . . no
C4 C5 1.377(4) . . no
C4 C7 1.506(5) . . no
C5 C6 1.377(4) . . no
C8 C9 1.525(3) . . no
C8 C14 1.486(3) . . no
C9 C10 1.518(4) . . no
C10 C11 1.535(4) . . no
C11 C12 1.490(5) . . no
C14 C15 1.398(3) . . no
C14 C19 1.403(3) . . no
C15 C16 1.382(3) . . no
C16 C17 1.383(3) . . no
C17 C18 1.408(3) . . no
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C9 H9' 0.9700 . . no
C10 H10 0.9700 . . no
C10 H10' 0.9700 . . no
C11 H11 0.9700 . . no
C11 H11' 0.9700 . . no
C13 H13 0.9600 . . no
C13 H13' 0.9600 . . no
C13 H13" 0.9600 . . no

C15 H15 0.9300 . . no
 C16 H16 0.9300 . . no
 C19 H19 0.9300 . . no
 C21 H21 0.9300 . . no
 C22 H22 0.9300 . . no
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 C27 H27 0.9700 . . no
 C27 H27' 0.9700 . . no
 C28 H28 0.9700 . . no
 C28 H28' 0.9700 . . no
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 C29 H29' 0.9700 . . no
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 C37 H37 0.9700 . . no
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 C38 H38 0.9600 . . no
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 O1 S1 N1 103.06(11) . . . yes
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 O2 S1 N1 108.60(11) . . . yes
 O2 S1 C1 108.48(11) . . . yes
 N1 S1 C1 107.13(11) . . . yes
 C12 O4 C13 116.7(2) . . . yes
 S1 N1 N2 117.52(14) . . . yes
 N1 N2 C8 115.84(18) . . . yes
 S1 N1 H1 121.00 . . . no
 N2 N1 H1 121.00 . . . no
 S1 C1 C2 119.8(2) . . . yes
 S1 C1 C6 120.80(18) . . . yes
 C2 C1 C6 119.4(2) . . . no
 C1 C2 C3 120.3(3) . . . no
 C2 C3 C4 121.1(3) . . . no
 C3 C4 C7 120.7(3) . . . no
 C5 C4 C7 121.5(3) . . . no
 C3 C4 C5 117.8(3) . . . no
 C4 C5 C6 121.6(3) . . . no
 C1 C6 C5 119.8(2) . . . no
 N2 C8 C9 122.9(2) . . . yes
 C9 C8 C14 119.80(19) . . . no

N2 C8 C14 117.3(2) . . . yes
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 C10 C11 C12 112.7(2) . . . no
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 C24 C25 C26 128.9(2) . . . no
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 C25 C26 C33 111.80(19) . . . no
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 C18 C26 C27 113.23(19) . . . no
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 C26 C27 C28 117.33(19) . . . no
 C27 C28 C29 112.0(2) . . . no
 C28 C29 C30 118.3(3) . . . no
 C29 C30 C31 112.8(3) . . . no
 C30 C31 C32 121.3(4) . . . no
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 C9 C10 H10 109.00 . . . no
 C9 C10 H10' 109.00 . . . no

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C11	C10	H10'	109.00	.	.	.	no
H10	C10	H10'	108.00	.	.	.	no
C10	C11	H11	109.00	.	.	.	no
C10	C11	H11'	109.00	.	.	.	no
C12	C11	H11	109.00	.	.	.	no
C12	C11	H11'	109.00	.	.	.	no
H11	C11	H11'	108.00	.	.	.	no
O4	C13	H13	109.00	.	.	.	no
O4	C13	H13'	109.00	.	.	.	no
O4	C13	H13"	110.00	.	.	.	no
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H13	C13	H13"	110.00	.	.	.	no
H13'	C13	H13"	110.00	.	.	.	no
C14	C15	H15	119.00	.	.	.	no
C16	C15	H15	119.00	.	.	.	no
C15	C16	H16	121.00	.	.	.	no
C17	C16	H16	121.00	.	.	.	no
C14	C19	H19	120.00	.	.	.	no
C18	C19	H19	120.00	.	.	.	no
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C28	C27	H27'	108.00	.	.	.	no
H27	C27	H27'	107.00	.	.	.	no
C27	C28	H28	109.00	.	.	.	no
C27	C28	H28'	109.00	.	.	.	no
C29	C28	H28	109.00	.	.	.	no
C29	C28	H28'	109.00	.	.	.	no
H28	C28	H28'	108.00	.	.	.	no
C28	C29	H29	108.00	.	.	.	no
C28	C29	H29'	108.00	.	.	.	no
C30	C29	H29	108.00	.	.	.	no
C30	C29	H29'	108.00	.	.	.	no
H29	C29	H29'	107.00	.	.	.	no
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C29	C30	H30'	109.00	.	.	.	no
C31	C30	H30	109.00	.	.	.	no
C31	C30	H30'	109.00	.	.	.	no
H30	C30	H30'	108.00	.	.	.	no
C30	C31	H31	107.00	.	.	.	no
C30	C31	H31'	107.00	.	.	.	no
C32	C31	H31	107.00	.	.	.	no
C32	C31	H31'	107.00	.	.	.	no
H31	C31	H31'	107.00	.	.	.	no
C31	C32	H32	109.00	.	.	.	no
C31	C32	H32'	109.00	.	.	.	no
C31	C32	H32"	110.00	.	.	.	no
H32	C32	H32'	109.00	.	.	.	no
H32	C32	H32"	109.00	.	.	.	no
H32'	C32	H32"	110.00	.	.	.	no
C26	C33	H33	108.00	.	.	.	no
C26	C33	H33'	108.00	.	.	.	no
C34	C33	H33	108.00	.	.	.	no
C34	C33	H33'	108.00	.	.	.	no
H33	C33	H33'	107.00	.	.	.	no
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C33	C34	H34'	109.00	.	.	.	no

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C36 C37 H37' 109.00 . . . no
C38 C37 H37 109.00 . . . no
C38 C37 H37' 109.00 . . . no
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C37 C38 H38 109.00 . . . no
C37 C38 H38' 109.00 . . . no
C37 C38 H38" 109.00 . . . no
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H38 C38 H38" 109.00 . . . no
H38' C38 H38" 109.00 . . . no

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O1 S1 N1 N2 -176.87(17) . . . . no
O2 S1 N1 N2 -47.5(2) . . . . no
C1 S1 N1 N2 69.45(19) . . . . no
O1 S1 C1 C2 -45.5(3) . . . . no
O1 S1 C1 C6 134.5(2) . . . . no
O2 S1 C1 C2 -178.0(2) . . . . no
O2 S1 C1 C6 1.9(2) . . . . no
N1 S1 C1 C2 64.9(2) . . . . no
N1 S1 C1 C6 -115.2(2) . . . . no
C13 O4 C12 O3 0.6(4) . . . . no
C13 O4 C12 C11 -177.8(2) . . . . no
S1 N1 N2 C8 -170.98(17) . . . . no
N1 N2 C8 C9 0.8(3) . . . . no
N1 N2 C8 C14 -179.30(19) . . . . no
S1 C1 C2 C3 -179.4(2) . . . . no
C6 C1 C2 C3 0.6(4) . . . . no
S1 C1 C6 C5 179.5(2) . . . . no
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C3 C4 C5 C6 0.0(5) . . . . no
C7 C4 C5 C6 -178.6(3) . . . . no
C4 C5 C6 C1 0.3(4) . . . . no
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N2 C8 C14 C15 -166.9(2) . . . . no
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C25 C20 C21 C22 0.6(4) . . . . no
C17 C20 C25 C24 -179.7(2) . . . . no
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 O2 C5 3.277(3) . 2_565 no
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 O2 H6 2.7600 . 2_565 no
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C6 H6 O2 0.9300 2.5500 2.921(3) 104.00 . yes

#===END of Crystallographic Information File

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