checkCIF/PLATON report

No syntax errors found.  CIF dictionary  Interpreting this report

Datablock: 1

Bond precision:  C-C = 0.0023 Å  Wavelength=0.7107 Å

Cell:  a=11.413(2)  b=9.0487(18)  c=7.1954(14)  
       alpha=90  beta=100.38(3)  gamma=90

Temperature:  173 K

<table>
<thead>
<tr>
<th>Calculated</th>
<th>Reported</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume</td>
<td>730.9(3)</td>
</tr>
<tr>
<td>Space group</td>
<td>P 21/c</td>
</tr>
<tr>
<td>Hall group</td>
<td>-P 2ybc</td>
</tr>
<tr>
<td>Moiety formula</td>
<td>C10 H6 O6 S2, 2(H3 O), 2(H2 O)</td>
</tr>
<tr>
<td>Sum formula</td>
<td>C10 H16 O10 S2</td>
</tr>
<tr>
<td>Mr</td>
<td>360.37</td>
</tr>
<tr>
<td>Dx, g cm⁻³</td>
<td>1.638</td>
</tr>
<tr>
<td>Z</td>
<td>2</td>
</tr>
<tr>
<td>M (mm⁻¹)</td>
<td>0.414</td>
</tr>
<tr>
<td>F(000)</td>
<td>376.0</td>
</tr>
<tr>
<td>F(000)‘</td>
<td>376.75</td>
</tr>
<tr>
<td>h, k, lmax</td>
<td>13, 10, 8</td>
</tr>
<tr>
<td>Nref</td>
<td>1361</td>
</tr>
<tr>
<td>Tmin, Tmax</td>
<td>0.876, 0.988</td>
</tr>
<tr>
<td>Tmin‘</td>
<td>0.876</td>
</tr>
</tbody>
</table>

Correction method= AbsCorr=INTEGRATION

Data completeness= Ratio = 0.983  Theta(max)= 25.490

R(reflections)= 0.0333(1251)  wR²(reflections)= 0.0905(1338)

S = 1.075  Npar = 115

The following ALERTS were generated. Each ALERT has the format

    test-name_ALERT_alert-type_alert-level

Click on the hyperlinks for more details of the test.

**Alert level B**

| PLAT417_ALERT_2_B | Short Inter D-H..H-D | H1A | .. | H2C | .. | 2.09 Ång. |

**Alert level C**

| ABSTY02_ALERT_1_C | An _exptl_absorpt_correction_type has been given without |
a literature citation. This should be contained in the _exptl_absorpt_process_details field.

Absorption correction given as integration

PLAT313_ALERT 2 C Oxygen with three covalent bonds (rare) ........ O2W
PLAT417_ALERT 2 C Short Inter D-H..H-D H1B .. H2C .. 2.10 Ang.

Alert level G

PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints ........ 9

ALERT level A = In general: serious problem
ALERT level B = Potentially serious problem
ALERT level C = Check and explain
ALERT level G = General alerts; check

ALERT type 1 CIF construction/syntax error, inconsistent or missing data
ALERT type 2 Indicator that the structure model may be wrong or deficient
ALERT type 3 Indicator that the structure quality may be low
ALERT type 4 Improvement, methodology, query or suggestion
ALERT type 5 Informative message, check

Datablock: 2

Bond precision:  C-C = 0.0033 Å  Wavelength=0.71073

Cell:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Calculated</th>
<th>Reported</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>12.8947(6) Å</td>
<td>12.8947(6) Å</td>
</tr>
<tr>
<td>b</td>
<td>6.9936(3) Å</td>
<td>6.9936(3) Å</td>
</tr>
<tr>
<td>c</td>
<td>15.6410(4) Å</td>
<td>15.6410(4) Å</td>
</tr>
<tr>
<td>alpha</td>
<td>90 °</td>
<td>90 °</td>
</tr>
<tr>
<td>beta</td>
<td>98.775(3) °</td>
<td>98.775(3) °</td>
</tr>
<tr>
<td>gamma</td>
<td>90 °</td>
<td>90 °</td>
</tr>
<tr>
<td>Temperature</td>
<td>173 K</td>
<td>173 K</td>
</tr>
</tbody>
</table>

Volume: 1394.00(10) Å³
Space group: P 21
Hall group: P 2yb
Moiety formula: C10 H6 O6 S2, 2(C8 H12 N), 2(H2 O)
Sum formula: C26 H34 N2 O8 S2
Mr: 566.69
Dx,g cm⁻³: 1.350
Z: 2
μ (mm⁻¹): 0.242
F000: 600.0
F000': 600.79
h,k,lmax: 17, 9, 20
Nref: 3647 (6748)
Tmin, Tmax: 0.880, 0.964
Tmin': 0.880

Correction method= AbsCorr=INTEGRATION
Data completeness = 1.83(0.99)  Theta(max) = 28.000
R(reflections) = 0.0354(6009)  wr2(reflections) = 0.0925(6675)
S = 1.060  Npar = 359

The following ALERTS were generated. Each ALERT has the format:
  test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

**Alert level C**

**ABSTY02_ALERT_1_C**  An _exptl_absorpt_correction_type has been given without a literature citation. This should be contained in the _exptl_absorpt_process_details field.

  Absorption correction given as integration

**PLAT221_ALERT_4_C**  Large Solvent/Anion C Ueq(max)/Ueq(min) ... 3.09 Ratio

**PLAT223_ALERT_4_C**  Large Solvent/Anion H Ueq(max)/Ueq(min) ... 3.12 Ratio

**PLAT250_ALERT_2_C**  Large U3/U1 Ratio for Average U(i,j) Tensor ..... 3.13

**PLAT731_ALERT_1_C**  Bond Calc 0.94(2), Rep 0.942(9) ...... 2.22 su-Ra

  O2W -H3W 1.555 1.555

**PLAT735_ALERT_1_C**  D-H Calc 0.94(2), Rep 0.942(9) ...... 2.22 su-Ra

  O2W -H3W 1.555 1.555

**PLAT790_ALERT_4_C**  Centre of Gravity not Within Unit Cell: Resd. # 4

  H2  O

**Alert level G**

**REFLT03_ALERT_4_G**  Please check that the estimate of the number of Friedel pairs is correct. If it is not, please give the correct count in the _publ_section_exptl_refinement section of the submitted CIF.

  From the CIF: _diffrn_reflns_theta_max 28.00
  From the CIF: _reflns_number_total 6675

  Count of symmetry unique reflns 3647
  Completeness (_total/calc) 183.03%
  TEST3: Check Friedels for noncentro structure
  Estimate of Friedel pairs measured 3028
  Fraction of Friedel pairs measured 0.830
  Are heavy atom types Z>Si present yes

**PLAT791_ALERT_1_G**  Confirm the Absolute Configuration of C16A ... R

**PLAT791_ALERT_1_G**  Confirm the Absolute Configuration of C16B ... R

**PLAT800_ALERT_4_G**  Note: Number of Least-Squares Restraints ....... 7

0 ALERT level A = In general: serious problem
0 ALERT level B = Potentially serious problem
7 ALERT level C = Check and explain
4 ALERT level G = General alerts; check

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Datablock: 3
Bond precision: C-C = 0.0047 Å

Wavelength = 0.71073 Å

Cell:
\[ a = 12.9026(10) \quad b = 7.0112(4) \quad c = 15.6618(13) \]
\[ \alpha = 90^\circ \quad \beta = 98.626(3) \quad \gamma = 90^\circ \]

Temperature: 173 K

<table>
<thead>
<tr>
<th>Calculated</th>
<th>Reported</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume</td>
<td>1400.78(18)</td>
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<tr>
<td>Space group</td>
<td>P 2 1</td>
</tr>
<tr>
<td>Hall group</td>
<td>P 2 y b</td>
</tr>
<tr>
<td>Moiety formula</td>
<td>C10 H6 O6 S2, 2(C8 H12 N), 2(H2 O)</td>
</tr>
<tr>
<td>Sum formula</td>
<td>C26 H34 N2 O8 S2</td>
</tr>
<tr>
<td>Mr</td>
<td>566.69</td>
</tr>
<tr>
<td>( \text{Dx, g cm}^{-3} )</td>
<td>1.344</td>
</tr>
<tr>
<td>Z</td>
<td>2</td>
</tr>
<tr>
<td>Mu (mm(^{-1}))</td>
<td>0.240</td>
</tr>
<tr>
<td>( F_{000} )</td>
<td>600.0</td>
</tr>
<tr>
<td>( F_{000}' )</td>
<td>600.79</td>
</tr>
<tr>
<td>( h,k,l_{\text{max}} )</td>
<td>17,9,20</td>
</tr>
<tr>
<td>Nref</td>
<td>3661(6776)</td>
</tr>
<tr>
<td>Tmin, Tmax</td>
<td>0.960,0.981</td>
</tr>
<tr>
<td>Tmin'</td>
<td>0.933</td>
</tr>
</tbody>
</table>

Correction method = AbsCorr=INTEGRATION

Data completeness = 1.84(0.99)
Theta(max) = 28.000

\[ R(\text{reflections}) = 0.0469(4498) \quad \text{wR}^2(\text{reflections}) = 0.1124(6720) \]

\[ S = 1.025 \quad \text{Npar} = 353 \]

The following ALERTS were generated. Each ALERT has the format
\[ \text{test-name}_ALERT\_alert-type_alert-level. \]
Click on the hyperlinks for more details of the test.

**Alert level C**

**ABSTY02_ALERT_1_C** An _exptl_absorpt_correction_type has been given without a literature citation. This should be contained in the _exptl_absorpt_process_details field.

Absorption correction given as integration

**PLAT231_ALERT_4_C** Hirshfeld Test (Solvent) C12B - C13B .. 5.15 su

**PLAT243_ALERT_4_C** High ‘Solvent’ Ueq as Compared to Neighbors for C13B

**PLAT250_ALERT_2_C** Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.81

**PLAT340_ALERT_3_C** Low Bond Precision on C-C Bonds (x 1000) Ang ... 5

**PLAT790_ALERT_4_C** Centre of Gravity not Within Unit Cell: Resd. # 4

**Alert level G**
Please check that the estimate of the number of Friedel pairs is correct. If it is not, please give the correct count in the _publ_section_exptl_refinement section of the submitted CIF.

From the CIF: _diffrn_reflns_theta_max 28.00
From the CIF: _reflns_number_total 6720
Count of symmetry unique reflns 3661
Completeness (_total/calc) 183.56%

TEST3: Check Friedels for noncentro structure
Estimate of Friedel pairs measured 3059
Fraction of Friedel pairs measured 0.836
Are heavy atom types Z>Si present yes

PLAT791_ALERT_1_G Confirm the Absolute Configuration of C16A ... S
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C16B ... S
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints ...... 7

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0 ALERT level A = In general: serious problem
0 ALERT level B = Potentially serious problem
6 ALERT level C = Check and explain
4 ALERT level G = General alerts; check

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 ALERT Type 2 Indicator that the structure model may be wrong or deficient
2 ALERT Type 3 Indicator that the structure quality may be low
4 ALERT Type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

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Datablock: 4

Bond precision:  C-C = 0.0023 A
Wavelength=0.71073

Cell:

\[ \begin{align*}
a &= 6.9709(5) \\
b &= 9.3885(7) \\
c &= 11.5361(7) \\
\alpha &= 68.520(4) \\
\beta &= 79.357(3) \\
\gamma &= 87.696(3)
\end{align*} \]

Temperature: 173 K

<table>
<thead>
<tr>
<th>Calculated</th>
<th>Reported</th>
</tr>
</thead>
<tbody>
<tr>
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<td>690.16(9)</td>
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<tr>
<td>Space group</td>
<td>P -1</td>
</tr>
<tr>
<td>Hall group</td>
<td>-P 1</td>
</tr>
<tr>
<td>Moiety formula</td>
<td>C10 H6 O6 S2, 2(C8 H12 N), C10 H6 O6 S2, 2(C8 H12 N), 2(H2 O)</td>
</tr>
<tr>
<td>Sum formula</td>
<td>C26 H34 N2 O8 S2</td>
</tr>
<tr>
<td>Mr</td>
<td>566.69</td>
</tr>
<tr>
<td>D, g cm(^{-3})</td>
<td>1.363</td>
</tr>
<tr>
<td>Z</td>
<td>1</td>
</tr>
<tr>
<td>Mu (mm(^{-1}))</td>
<td>0.244</td>
</tr>
<tr>
<td>F000</td>
<td>300.00</td>
</tr>
<tr>
<td>F000'</td>
<td>300.39</td>
</tr>
<tr>
<td>h,k,lmax</td>
<td>9,12,15</td>
</tr>
<tr>
<td>Nref</td>
<td>3330</td>
</tr>
<tr>
<td>Tmin,Tmax</td>
<td>0.920, 0.964</td>
</tr>
<tr>
<td>Tmin’</td>
<td>0.920</td>
</tr>
</tbody>
</table>
Correction method = AbsCorr=INTEGRATION

Data completeness = Ratio = 0.997    Theta(max)= 28.000

R(reflections)= 0.0357( 2864)     wR2(reflections)= 0.0967( 3320)

S = 1.063            Npar= 180

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

**Alert level C**

**ABSTY02_ALERT_1_C** An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.
Absorption correction given as integration

**PLAT152_ALERT_1_C** Supplied and Calc Volume s.u. Inconsistent .....          ?

**PLAT731_ALERT_1_C** Bond Calc 0.93(2), Rep 0.931(9) ......       2.22 su-Ra
  O1W -H2W 1.555 1.555

**PLAT735_ALERT_1_C** D-H Calc 0.93(2), Rep 0.931(9) ......       2.22 su-Ra
  O1W -H2W 1.555 1.555

**Alert level G**

**PLAT793_ALERT_2_G** Check the Absolute Configuration of C16    .....          S

**PLAT860_ALERT_3_G** Note: Number of Least-Squares Restraints .......          3

0 ALERT level A = In general: serious problem
0 ALERT level B = Potentially serious problem
4 ALERT level C = Check and explain
2 ALERT level G = General alerts; check

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

**Datablock: 5**

**Bond precision:**    C-C = 0.0042 A

**Wavelength**=0.71073

**Cell:**
  a=10.6886(3) b=11.2210(3) c=21.3919(7)
  alpha=90    beta=93.741(2)    gamma=90

**Temperature:**  173 K
Calculated Reported

<table>
<thead>
<tr>
<th>Property</th>
<th>Calculated</th>
<th>Reported</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume</td>
<td>2560.21(13)</td>
<td>2560.21(13)</td>
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<tr>
<td>Space group</td>
<td>P 2</td>
<td>P2</td>
</tr>
<tr>
<td>Hall group</td>
<td>P 2y</td>
<td>P 2y</td>
</tr>
<tr>
<td>Moiety formula</td>
<td>C10 H6 O6 S2, 2(C8 H12 N)</td>
<td>C10 H6 O6 S2, 2(C8 H12 N)</td>
</tr>
<tr>
<td>Sum formula</td>
<td>C26 H30 N2 O6 S2</td>
<td>C26 H30 N2 O6 S2</td>
</tr>
<tr>
<td>Mr</td>
<td>530.66</td>
<td>530.64</td>
</tr>
<tr>
<td>Dx, g cm⁻³</td>
<td>1.377</td>
<td>1.377</td>
</tr>
<tr>
<td>Z</td>
<td>4</td>
<td>4</td>
</tr>
<tr>
<td>Mu (mm⁻¹)</td>
<td>0.252</td>
<td>0.252</td>
</tr>
<tr>
<td>F₀₀₀</td>
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<td>1120.0</td>
</tr>
<tr>
<td>F₀₀₀'</td>
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<td></td>
</tr>
<tr>
<td>h,k,lmax</td>
<td>14,14,28</td>
<td>14,14,28</td>
</tr>
<tr>
<td>Nref</td>
<td>6500 (12373)</td>
<td>12320</td>
</tr>
<tr>
<td>Tmin, Tmax</td>
<td>0.939, 0.985</td>
<td>0.928, 0.985</td>
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<tr>
<td>Tmin’</td>
<td>0.939</td>
<td></td>
</tr>
</tbody>
</table>

Correction method = AbsCorr=INTEGRATION

Data completeness = 1.90 (1.00)  Theta(max) = 28.000

R(reflections) = 0.0430 (8317)  wR²(reflections) = 0.0985 (12320)

S = 0.975  Npar = 657

The following ALERTS were generated. Each ALERT has the format test-name_ALERT_alert-type_alert-level. Click on the hyperlinks for more details of the test.

**Alert level B**
PLAT111_ALERT_2_B ADDSYM Detects (Pseudo) Centre of Symmetry ..... 94 PerFi

**Alert level C**
ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without a literature citation. This should be contained in the _exptl_absorpt_process_details field. Absorption correction given as integration
PLAT113_ALERT_2_C ADDSYM Suggests Possible Pseudo/New Space-group. P2/c
PLAT430_ALERT_2_C Short Inter D...A Contact 07 .. 07 .. 2.88 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 3 C8 H12 N
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 4 C8 H12 N

**Alert level G**
REFLT03_ALERT_4_G Please check that the estimate of the number of Friedel pairs is correct. If it is not, please give the correct count in the _publ_section_exptl_refinement section of the submitted CIF.
From the CIF: _diffrn_reflns_theta_max 28.00
From the CIF: _reflns_number_total 12320
Count of symmetry unique reflns          6500
Completeness (_total/calc)                189.54%
TEST3: Check Friedels for noncentro structure
Estimate of Friedel pairs measured       5820
Fraction of Friedel pairs measured       0.895
Are heavy atom types Z>Si present        yes

PLAT791_ALERT_1_G Confirm the Absolute Configuration of C16A ...  R
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C16B ...  R
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C16C ...  R
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C16D ...  R
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......  1

ALERT level A = In general: serious problem
ALERT level B = Potentially serious problem
ALERT level C = Check and explain
ALERT level G = General alerts; check

ALERT type 1 CIF construction/syntax error, inconsistent or missing data
ALERT type 2 Indicator that the structure model may be wrong or deficient
ALERT type 3 Indicator that the structure quality may be low
ALERT type 4 Improvement, methodology, query or suggestion
ALERT type 5 Informative message, check

Datablock: 6

Bond precision:  C-C = 0.0039 A    Wavelength=0.71073

Cell:    a=10.6875(3)    b=11.2208(2)    c=21.4087(7)
         alpha=90          beta=93.765(1)    gamma=90
Temperature:  173 K

Volume        2561.84(12) 2561.84(12)
Space group   P 2      P2
Hall group    P 2y     P 2y
Moiety formula C10 H6 O6 S2, 2(C8 H12 N) C10 H6 O6 S2, 2(C8 H12 N)
Sum formula   C26 H30 N2 O6 S2 C26 H30 N2 O6 S2
Mr            530.66    530.64
Dx, g cm−3    1.376     1.376
Z              4         4
Mu (mm−1)     0.252     0.252
F000          1120.0    1120.0
F000’         1121.50   1121.50
h,k,l max    14,14,28   14,14,28
Nref          6507(12386) 12360
Tmin, Tmax    0.911, 0.985 0.895, 0.985
Tmin’         0.868

Correction method= AbsCorr=INTEGRATION
Data completeness = 1.90(1.00)  Theta(max) = 28.000

R(reflections) = 0.0435(8931)  wR2(reflections) = 0.1028(12360)

S = 0.992  Npar = 657

The following ALERTS were generated. Each ALERT has the format

  test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

**Alert level B**

<table>
<thead>
<tr>
<th>ALERT</th>
<th>Description</th>
<th>Alert level</th>
</tr>
</thead>
<tbody>
<tr>
<td>PLAT111_ALERT_2_B</td>
<td>ADDSYM Detects (Pseudo) Centre of Symmetry</td>
<td>94 PerFi</td>
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**Alert level C**

<table>
<thead>
<tr>
<th>ALERT</th>
<th>Description</th>
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<tbody>
<tr>
<td>ABSTY02_ALERT_1_C</td>
<td>An _exptl_absorp_correction_type has been given without a literature citation. This should be contained in the _exptl_absorp_process_details field. Absorption correction given as integration</td>
</tr>
<tr>
<td>PLAT113_ALERT_2_C</td>
<td>ADDSYM Suggests Possible Pseudo/New Space-group. P2/c</td>
</tr>
<tr>
<td>PLAT430_ALERT_2_C</td>
<td>Short Inter D...A Contact  O7 .. O7 .. 2.88 Ang.</td>
</tr>
<tr>
<td>PLAT790_ALERT_4_C</td>
<td>Centre of Gravity not Within Unit Cell: Resd. # 3  C8 H12 N</td>
</tr>
<tr>
<td>PLAT790_ALERT_4_C</td>
<td>Centre of Gravity not Within Unit Cell: Resd. # 4  C8 H12 N</td>
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**Alert level G**

<table>
<thead>
<tr>
<th>ALERT</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>REFLT03_ALERT_4_G</td>
<td>Please check that the estimate of the number of Friedel pairs is correct. If it is not, please give the correct count in the _publ_section_exptl_refinement section of the submitted CIF.</td>
</tr>
<tr>
<td>PLAT791_ALERT_1_G</td>
<td>Confirm the Absolute Configuration of C16A ... S</td>
</tr>
<tr>
<td>PLAT791_ALERT_1_G</td>
<td>Confirm the Absolute Configuration of C16B ... S</td>
</tr>
<tr>
<td>PLAT791_ALERT_1_G</td>
<td>Confirm the Absolute Configuration of C16C ... S</td>
</tr>
<tr>
<td>PLAT791_ALERT_1_G</td>
<td>Confirm the Absolute Configuration of C16D ... S</td>
</tr>
<tr>
<td>PLAT860_ALERT_3_G</td>
<td>Note: Number of Least-Squares Restraints ....... 1</td>
</tr>
</tbody>
</table>

0 ALERT level A = In general: serious problem
1 ALERT level B = Potentially serious problem
5 ALERT level C = Check and explain
6 ALERT level G = General alerts; check

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check
Datablock: 7

Bond precision:  C-C = 0.0023 Å  Wavelength=0.71073

Cell:

\[
\begin{align*}
a &= 20.9153(9) & b &= 11.1980(5) & c &= 10.7591(5) \\
a &= 20.9153(9) & b &= 11.1980(5) & c &= 10.7591(5) \\
\alpha &= 90 & \beta &= 90 & \gamma &= 90 \\
\alpha &= 90 & \beta &= 90 & \gamma &= 90 \\
\end{align*}
\]

Temperature: 173 K

Calculated  Reported

| Volume | 2519.9(2) | 2519.9(2) |
| Space group | P b c n | Pbcn |
| Hall group | -P 2n 2ab | -P 2n 2ab |
| Moiety formula | C10 H6 O6 S2, 2(C8 H12 N) | C10 H6 O6 S2, 2(C8 H12 N) |
| Sum formula | C26 H30 N2 O6 S2 | C26 H30 N2 O6 S2 |
| Mr | 530.66 | 530.64 |
| Dx,g cm\(^{-3}\) | 1.399 | 1.399 |
| Z | 4 | 4 |
| Mu (mm\(^{-1}\)) | 0.257 | 0.257 |
| F000 | 1120.0 | 1120.0 |
| F000' | 1121.50 |
| h,k,lmax | 27,14,14 | 27,14,14 |
| Nref | 3045 | 3043 |
| Tmin, Tmax | 0.879,0.990 | 0.904,0.990 |
| Tmin' | 0.879 |

Correction method= AbsCorr=INTEGRATION

Data completeness= Ratio = 0.999  Theta(max)= 27.990

R(reflections)= 0.0366( 2244)  wR2(reflections)= 0.0953( 3043)

\[ S = 1.039 \quad Npar= 165 \]

The following ALERTS were generated. Each ALERT has the format

\textit{test-name_ALERT_alert-type_alert-level}

Click on the hyperlinks for more details of the test.

** Alert level C  
\text{ABSTY02_ALERT_1_C}  
An _exptl_absorpt_correction_type has been given without a literature citation. This should be contained in the _exptl_absorpt_process_details field.  
Absorption correction given as integration

** Alert level G  
\text{PLAT793_ALERT_2_G}  
Check the Absolute Configuration of C16       .......  S

0 ALERT level A = In general: serious problem
0 ALERT level B = Potentially serious problem
1 ALERT level C = Check and explain
1 ALERT level G = General alerts; check

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

---

**Datablock: 8**

**Bond precision:**  C-C = 0.0083 Å  
**Wavelength=0.71073**

**Cell:**
- a=5.9861(5)
- b=7.5878(5)
- c=18.2064(16)
- alpha=89.152(4)
- beta=81.962(4)
- gamma=89.104(5)

**Temperature:**  173 K

<table>
<thead>
<tr>
<th></th>
<th>Calculated</th>
<th>Reported</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Volume</strong></td>
<td>818.67(11)</td>
<td>818.67(11)</td>
</tr>
<tr>
<td><strong>Space group</strong></td>
<td>P 1</td>
<td>P1</td>
</tr>
<tr>
<td><strong>Hall group</strong></td>
<td>P 1</td>
<td>P1</td>
</tr>
<tr>
<td><strong>Moiety formula</strong></td>
<td>C10 H7 O3 S, C8 H12 N</td>
<td>C10 H7 O3 S, C8 H12 N</td>
</tr>
<tr>
<td><strong>Sum formula</strong></td>
<td>C18 H19 N O3 S</td>
<td>C18 H19 N O3 S</td>
</tr>
<tr>
<td><strong>Mr</strong></td>
<td>329.41</td>
<td>329.40</td>
</tr>
<tr>
<td><strong>Dx,g cm(^{-3})</strong></td>
<td>1.336</td>
<td>1.336</td>
</tr>
<tr>
<td><strong>Z</strong></td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td><strong>Mu (mm(^{-1}))</strong></td>
<td>0.212</td>
<td>0.212</td>
</tr>
<tr>
<td><strong>F000</strong></td>
<td>348.0</td>
<td>348.0</td>
</tr>
<tr>
<td><strong>F000’</strong></td>
<td>348.40</td>
<td></td>
</tr>
<tr>
<td><strong>h,k,lmax</strong></td>
<td>7, 9, 22</td>
<td>7, 9, 22</td>
</tr>
<tr>
<td><strong>Nref</strong></td>
<td>3046( 6092)</td>
<td>5915</td>
</tr>
<tr>
<td><strong>Tmin,Tmax</strong></td>
<td>0.936, 0.992</td>
<td>0.870, 0.992</td>
</tr>
<tr>
<td><strong>Tmin’</strong></td>
<td>0.898</td>
<td></td>
</tr>
</tbody>
</table>

**Correction method= AbsCorr=INTEGRATION**

**Data completeness= 1.94(0.97)**  
**Theta(max)= 25.500**

**R(reflections)= 0.0537( 4563)**  
**wR2(reflections)= 0.1171( 5915)**

**S = 0.955**  
**Npar= 419**

---

The following ALERTS were generated. Each ALERT has the format  
**test-name_ALERT_alert-type_alert-level**.  
Click on the hyperlinks for more details of the test.

- Alert level B
Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without a literature citation. This should be contained in the _exptl_absorpt_process_details field.

Absorption correction given as integration

PLAT111_ALERT_2_C ADDSYM Detects (Pseudo) Centre of Symmetry ..... 95 PerFi

Alert level G

REFLT03_ALERT_4_G Please check that the estimate of the number of Friedel pairs is correct. If it is not, please give the correct count in the _publ_section_exptl_refinement section of the submitted CIF.

From the CIF: _diffrn_reflns_theta_max 25.50
From the CIF: _reflns_number_total 5915
Count of symmetry unique reflns 3046
Completeness (_total/calc) 194.19%
TEST3: Check Friedels for noncentro structure
Estimate of Friedel pairs measured 2869
Fraction of Friedel pairs measured 0.942
Are heavy atom types Z>Si present yes

PLAT791_ALERT_1_G Confirm the Absolute Configuration of C16A ... R
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C16B ... R
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints ........ 3

Datablock: 9

Bond precision:  C-C = 0.0058 A  Wavelength=0.71073

Cell: a=5.9629(3)  b=7.5551(4)  c=18.1340(9)
      alpha=89.131(2)  beta=81.986(2)  gamma=89.098(2)
Temperature: 173 K
### Summary

<table>
<thead>
<tr>
<th>Calculated</th>
<th>Reported</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Volume</strong></td>
<td>808.79(7)</td>
</tr>
<tr>
<td><strong>Space group</strong></td>
<td><strong>P 1</strong></td>
</tr>
<tr>
<td><strong>Hall group</strong></td>
<td><strong>P 1</strong></td>
</tr>
<tr>
<td><strong>Moiety formula</strong></td>
<td>C10 H7 O3 S, C8 H12 N</td>
</tr>
<tr>
<td><strong>Sum formula</strong></td>
<td>C18 H19 N O3 S</td>
</tr>
<tr>
<td><strong>Mr</strong></td>
<td>329.41</td>
</tr>
<tr>
<td><strong>Dx,g cm⁻³</strong></td>
<td>1.353</td>
</tr>
<tr>
<td><strong>Z</strong></td>
<td>2</td>
</tr>
<tr>
<td><strong>Mu (mm⁻¹)</strong></td>
<td>0.215</td>
</tr>
<tr>
<td><strong>F000</strong></td>
<td>348.0</td>
</tr>
<tr>
<td><strong>F000’</strong></td>
<td>348.40</td>
</tr>
<tr>
<td><strong>h,k,lmax</strong></td>
<td>7,9,21</td>
</tr>
<tr>
<td><strong>Nref</strong></td>
<td>3005 (6010)</td>
</tr>
<tr>
<td><strong>Tmin,Tmax</strong></td>
<td>0.965,0.987</td>
</tr>
</tbody>
</table>

**Correction method:** AbsCorr=INTEGRATION

**Data completeness:** 2.00(1.00)  \hspace{1cm} **Theta(max)** = 25.500

**R(reflections)** = 0.0434 (4808)  \hspace{1cm} **wR2(reflections)** = 0.1094 (6006)

**S = 0.899**  \hspace{1cm} **Npar = 419**

---

The following ALERTS were generated. Each ALERT has the format `test-name_ALERT_alert-type_alert-level`.

Click on the hyperlinks for more details of the test.

#### Alert level A

**DENSX01_ALERT_1_A**  
The ratio of the calculated to measured crystal density lies outside the range 0.80 <> 1.20  
Calculated density = 1.353  
Measured density = 0.000

#### Alert level B

**PLAT111_ALERT_2_B**  
ADDSYM Detects (Pseudo) Centre of Symmetry ..... 95 PerFi

#### Alert level C

**ABSTY02_ALERT_1_C**  
An _exptl_absorpt_correction_type has been given without a literature citation. This should be contained in the _exptl_absorpt_process_details field.  
Absorption correction given as integration

**PLAT113_ALERT_2_C**  
ADDSYM Suggests Possible Pseudo/New Space-group. P-1

**PLAT154_ALERT_1_C**  
The su’s on the Cell Angles are Equal (x 10000) 200 Deg.

**PLAT195_ALERT_1_C**  
Missing _cell_measurement_theta_max datum .... ?

**PLAT196_ALERT_1_C**  
Missing _cell_measurement_theta_min datum .... ?

**PLAT340_ALERT_3_C**  
Low Bond Precision on C-C Bonds (x 1000) Ang ... 6
Please check that the estimate of the number of Friedel pairs is correct. If it is not, please give the correct count in the _publ_section_exptl_refinement section of the submitted CIF.

From the CIF: _diffrn_reflns_theta_max 25.50
From the CIF: _reflns_number_total 6006
Count of symmetry unique reflns 3005
Completeness (_total/calc) 199.87%

TEST3: Check Friedels for noncentro structure
Estimate of Friedel pairs measured 3001
Fraction of Friedel pairs measured 0.999
Are heavy atom types Z>Si present yes

Confirm the Absolute Configuration of C16A ...
Confirm the Absolute Configuration of C16B ...

Note: Number of Least-Squares Restraints ........ 3

Datablock: 10

Bond precision:  C-C = 0.0039 Å  Wavelength=0.71073

Cell:  
\[ \begin{array}{ccc}
    a &=& 6.0783(6) \\
    b &=& 7.5053(5) \\
    c &=& 18.2131(18) \\
    \alpha &=& 86.341(6) \\
    \beta &=& 83.473(4) \\
    \gamma &=& 86.509(6)
\end{array} \]

Temperature:  173 K

<table>
<thead>
<tr>
<th>Property</th>
<th>Calculated</th>
<th>Reported</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume</td>
<td>822.60(13)</td>
<td>822.60(13)</td>
</tr>
<tr>
<td>Space group</td>
<td>P -1</td>
<td>P-1</td>
</tr>
<tr>
<td>Hall group</td>
<td>-P 1</td>
<td>-P 1</td>
</tr>
<tr>
<td>Moiety formula</td>
<td>C10 H7 O3 S, C8 H12 N</td>
<td>C10 H7 O3 S, C8 H12 N</td>
</tr>
<tr>
<td>Sum formula</td>
<td>C18 H19 N O3 S</td>
<td>C18 H19 N O3 S</td>
</tr>
<tr>
<td>Mr</td>
<td>329.41</td>
<td>329.40</td>
</tr>
<tr>
<td>(D_x, g \ cm^{-3})</td>
<td>1.330</td>
<td>1.330</td>
</tr>
<tr>
<td>(Z)</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>(\mu (\text{mm}^{-1}))</td>
<td>0.211</td>
<td>0.211</td>
</tr>
<tr>
<td>(F(000))</td>
<td>348.0</td>
<td>348.0</td>
</tr>
<tr>
<td>(F(000)’)</td>
<td>348.40</td>
<td></td>
</tr>
<tr>
<td>(h,k,l_{max})</td>
<td>7,9,22</td>
<td>7,9,22</td>
</tr>
<tr>
<td>(N_{ref})</td>
<td>3069</td>
<td>3014</td>
</tr>
<tr>
<td>(T_{min}, T_{max})</td>
<td>0.938, 0.988</td>
<td>0.893, 0.988</td>
</tr>
<tr>
<td>(T_{min}’)</td>
<td>0.900</td>
<td></td>
</tr>
</tbody>
</table>
Correction method= AbsCorr=INTEGRATION

Data completeness= Ratio = 0.982  Theta(max)= 25.500

R(reflections)= 0.0607( 2294)  wR2(reflections)= 0.1581( 3014)

S = 1.070  Npar= 210

The following ALERTS were generated. Each ALERT has the format test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

**Alert level C**

ABSTY02_ALERT_1_C  An _exptl_absorpt_correction_type has been given without a literature citation. This should be contained in the _exptl_absorpt_process_details field.
Absorption correction given as integration

PLAT250_ALERT_2_C  Large U3/U1 Ratio for Average U(i,j) Tensor ... 2.06

**Alert level G**

PLAT793_ALERT_2_G  Check the Absolute Configuration of C16 ...... S

0 ALERT level A = In general: serious problem
0 ALERT level B = Potentially serious problem
2 ALERT level C = Check and explain
1 ALERT level G = General alerts; check

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check
Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation); however, if you intend to submit to Acta Crystallographica Section C or E, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the Notes for Authors of the relevant journal for any special instructions relating to CIF submission.