checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: CCDC-1051179

```
Bond precision:   C-C = 0.0046 A           Wavelength=0.71073

Cell:            a=9.4587(5)      b=9.6256(4)       c=11.5993(6)
                 alpha=90         beta=90           gamma=90
Temperature:     150 K

                 Calculated                  Reported
Volume           1056.07(9)                  1056.07(9)
Space group      P 21 21 21                  P2(1)2(1)2(
Hall group       P 2ac 2ab                   ?
Moiety formula   C9 H10 O S3                 ?
Sum formula      C9 H10 O S3                 C9 H10 O S3
Mr               230.35                      230.35
Dx,g cm-3        1.449                       1.449
Z                4                           4
Mu (mm-1)        0.658                       0.658
F000             480.0                       480.0
F000'            481.62
h,k,lmax         11,11,13                    11,11,13
Nref             1910[ 1122]                 1897
Tmin,Tmax        0.854,0.936                 0.827,0.937
Tmin'            0.821

Correction method= # Reported T Limits: Tmin=0.827 Tmax=0.937
AbsCorr = MULTI-SCAN

Data completeness= 1.69/0.99      Theta(max)= 25.260

R(reflections)= 0.0329( 1690)      wR2(reflections)= 0.0793( 1897)

S = 1.075                Npar= 140
```

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
PLAT230_ALERT_2_B Hirshfeld Test Diff for   C6   -- C8   ..   7.3 su

Alert level C
PLAT213_ALERT_2_C Atom C4A   has ADP max/min Ratio .....   3.3 oblate
PLAT234_ALERT_4_C Large Hirshfeld Difference C5   -- C4   ..   0.17 Ang.
PLAT242_ALERT_2_C Low   Ueq as Compared to Neighbors for .....   C6 Check
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ....   0.0046 Ang.

Alert level G
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF   Please Do !
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical   ? Check
PLAT230_ALERT_2_G Hirshfeld Test Diff for   C4A   -- C5   ..   6.3 su
PLAT300_ALERT_4_G Atom Site Occupancy of >S3A   is Constrained at   0.511 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <S3   is Constrained at   0.489 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C4A   is Constrained at   0.511 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C4   is Constrained at   0.489 Check
PLAT301_ALERT_3_G Main Residue Disorder .... Percentage =   15 Note
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #   16 Check
          C4A -C2 -S3   1.555 1.555 1.555   14.80 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #   24 Check
          C4 -C3 -S3A   1.555 1.555 1.555   14.30 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #   30 Check
          C4 -C5 -S3A   1.555 1.555 1.555   17.20 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #   32 Check
          C4A -C5 -S3   1.555 1.555 1.555   13.80 Deg.
PLAT850_ALERT_4_G Check Flack Parameter Exact Value 0.00 and su ..   0.12 Check
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL   2014 Note

   0 **ALERT level A** = Most likely a serious problem - resolve or explain
   1 **ALERT level B** = A potentially serious problem, consider carefully
   4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
  14 **ALERT level G** = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   4 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
  11 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check

Datablock: CCDC-1051177

Bond precision: C-C = 0.0041 A   Wavelength=0.71073

Cell: a=9.9526(3)   b=12.2499(3)   c=17.9352(4)
             alpha=81.381(1)   beta=85.234(2)   gamma=89.204(1)
Temperature: 150 K

	Calculated	Reported
Volume	2154.46(10)	2154.46(10)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C18 H18 N2 S7	?
Sum formula	C18 H18 N2 S7	C18 H18 N2 S7
Mr	486.76	486.76
Dx,g cm-3	1.501	1.501
Z	4	4
Mu (mm-1)	0.739	0.739
F000	1008.0	1008.0
F000'	1011.67	
h,k,lmax	12,14,21	12,14,21
Nref	8173	8009
Tmin,Tmax	0.837,0.985	0.709,0.985
Tmin'	0.691	

Correction method= # Reported T Limits: Tmin=0.709 Tmax=0.985
AbsCorr = MULTI-SCAN

Data completeness= 0.980   Theta(max)= 25.680

R(reflections)= 0.0387(5668)   wR2(reflections)= 0.0904(8009)

S = 1.019   Npar= 599

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
```
PLAT213_ALERT_2_C Atom C3           has ADP max/min Ratio .....      3.3 prolat
PLAT213_ALERT_2_C Atom C21          has ADP max/min Ratio .....      3.4 prolat
PLAT220_ALERT_2_C Large Non-Solvent  C    Ueq(max)/Ueq(min) Range    4.3 Ratio
PLAT220_ALERT_2_C Large Non-Solvent  C    Ueq(max)/Ueq(min) Range    5.8 Ratio
PLAT222_ALERT_3_C Large Non-Solvent  H    Uiso(max)/Uiso(min) ...    5.3 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C5    -- C6A    ..     0.17 Ang.
PLAT241_ALERT_2_C High    Ueq as Compared to Neighbors for .....     S3 Check
PLAT241_ALERT_2_C High    Ueq as Compared to Neighbors for .....     S9 Check
PLAT242_ALERT_2_C Low     Ueq as Compared to Neighbors for .....     C1 Check
PLAT242_ALERT_2_C Low     Ueq as Compared to Neighbors for .....    C19 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............  0.0041 Ang.
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⚪ Alert level G
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PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...      3 Report
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF   Please Do !
PLAT230_ALERT_2_G Hirshfeld Test Diff for     C32    -- C33    ..     6.0 su
PLAT230_ALERT_2_G Hirshfeld Test Diff for     C35    -- C36    ..     6.0 su
PLAT300_ALERT_4_G Atom Site Occupancy of >S1    is Constrained at   0.709 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <S1A   is Constrained at   0.291 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >N2    is Constrained at   0.794 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of >C2     is Constrained at      0.725 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C3     is Constrained at      0.725 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C4     is Constrained at      0.725 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C6     is Constrained at      0.709 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C16    is Constrained at      0.794 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C17    is Constrained at      0.794 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C18    is Constrained at      0.794 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <N2A    is Constrained at      0.206 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C2A    is Constrained at      0.275 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C3A    is Constrained at      0.275 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C4A    is Constrained at      0.275 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C6A    is Constrained at      0.291 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C16A   is Constrained at      0.206 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C17A   is Constrained at      0.206 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C18A   is Constrained at      0.206 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >S8     is Constrained at      0.773 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <S8A    is Constrained at      0.227 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C24    is Constrained at      0.773 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C24A   is Constrained at      0.227 Check
PLAT301_ALERT_3_G Main Residue  Disorder ............ Percentage =         20 Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          9 Note
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #          8 Check
            C16A -S7  -C16    1.555   1.555   1.555           34.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         18 Check
            C2A  -C1  -C2     1.555   1.555   1.555           33.40 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         31 Check
            C4   -C1  -C4A    1.555   1.555   1.555           37.40 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         39 Check
            C6   -C5  -S1A    1.555   1.555   1.555           14.20 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         43 Check
            C6A  -C5  -S1     1.555   1.555   1.555           15.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         48 Check
            C6   -C7  -S1A    1.555   1.555   1.555           15.80 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         54 Check
            C6A  -C8  -S1     1.555   1.555   1.555           16.80 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        110 Check
            C24  -C23 -S8A    1.555   1.555   1.555           15.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        114 Check
            C24A -C23 -S8     1.555   1.555   1.555           12.90 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        119 Check
            C24  -C25 -S8A    1.555   1.555   1.555           14.40 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        125 Check
            C24A -C26 -S8     1.555   1.555   1.555           16.70 Deg.
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         24 Note
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL       2014 Note
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
  11 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  41 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  11 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 ALERT type 3 Indicator that the structure quality may be low
  36 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
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Datablock: CCDC-1051178

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Bond precision:   C-C = 0.0041 A            Wavelength=0.71073

Cell:          a=7.2530(1)        b=8.3877(1)        c=26.2705(4)
               alpha=86.235(1)    beta=86.176(1)     gamma=71.720(1)
Temperature:   150 K

                     Calculated                 Reported
Volume               1512.47(4)                 1512.47(4)
Space group          P -1                       P-1
Hall group           -P 1                       ?
Moiety formula       C15 H12 N2 S7, C8 Au N4 S4 C15 H12 N2 S7, C8 Au N4 S4
Sum formula          C23 H12 Au N6 S11          C23 H12 Au N6 S11
Mr                   922.02                     922.01
Dx,g cm-3            2.025                      2.025
Z                    2                          2
Mu (mm-1)            5.652                      5.652
F000                 894.0                      894.0
F000'                892.98
h,k,lmax             9,10,32                    9,10,32
Nref                 6181                       6102
Tmin,Tmax            0.513,0.798                0.211,0.805
Tmin'                0.103

Correction method= # Reported T Limits: Tmin=0.211 Tmax=0.805
AbsCorr = MULTI-SCAN

Data completeness= 0.987          Theta(max)= 26.370

R(reflections)= 0.0173( 6057)     wR2(reflections)= 0.0421( 6102)

S = 1.253                    Npar= 390
```

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
```
PLAT220_ALERT_2_C Large Non-Solvent  C     Ueq(max)/Ueq(min) Range       3.2 Ratio
```

⚪ Alert level G
```
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...        2 Report
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF    Please Do !
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal ..........  0.00100 Degree
PLAT230_ALERT_2_G Hirshfeld Test Diff for     S7     -- C12      ..        6.1 su
PLAT230_ALERT_2_G Hirshfeld Test Diff for     S7A    -- C12      ..        5.6 su
PLAT300_ALERT_4_G Atom Site Occupancy of >S7    is Constrained at    0.551 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <S7A   is Constrained at    0.449 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C11   is Constrained at    0.551 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C11A  is Constrained at    0.449 Check
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PLAT301_ALERT_3_G Main Residue  Disorder ........... Percentage =        5 Note
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #       35 Check
          C11A -C9   -S7     1.555   1.555   1.555           9.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #       41 Check
          C11  -C10  -S7A    1.555   1.555   1.555           9.70 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #       48 Check
          C11  -C12  -S7A    1.555   1.555   1.555          12.10 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #       52 Check
          C11A -C12  -S7     1.555   1.555   1.555          13.10 Deg.
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       12 Note
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL     2014 Note
```

```
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   9 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
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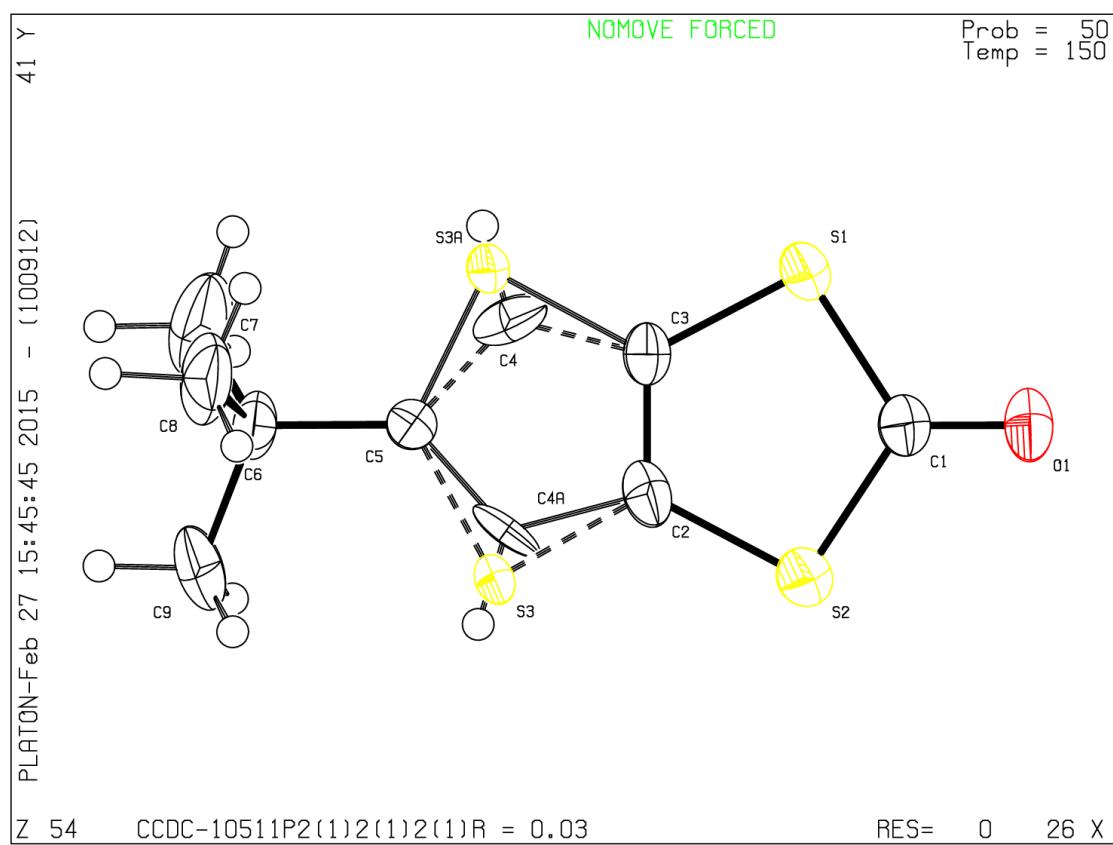
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

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.

PLATON version of 29/01/2015; check.def file version of 29/01/2015