checkCIF/PLATON report

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

No syntax errors found. CIF dictionary Interpreting this report

Datablock: I

```
Bond precision:  C-C = 0.0293 A          Wavelength=0.71073

Cell:            a=15.984(9)     b=20.991(12)       c=26.596(16)
                 alpha=90        beta=101.21(2)     gamma=90
Temperature:     100 K
```

	Calculated	Reported
Volume	8753(9)	8753(9)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C20 H40 N6 S2, 5(H2 O4 P), H2.01 O2.52 P0.51, H2 O1.98 P0.49, 0	C20 H58.51 N6 O26 P6 S2
Sum formula	C20 H58.51 N6 O26 P6 S2	C20 H58.51 N6 O26 P6 S2
Mr	1049.10	1049.10
Dx,g cm-3	1.592	1.592
Z	8	8
Mu (mm-1)	0.434	0.434
F000	4404.1	4404.1
F000’	4413.08	
h,k,lmax	14,19,24	14,19,24
Nref	3650	3647
Tmin,Tmax	0.823,0.844	0.825,0.846
Tmin’	0.823	

```
Correction method= MULTI-SCAN

Data completeness= 0.999          Theta(max)= 19.210

R(reflections)= 0.1513( 3387)     wR2(reflections)= 0.4086( 3647)

S = 1.347                 Npar= 606
```

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

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550

```
           Calculated sin(theta_max)/wavelength =    0.4629
PLAT023_ALERT_3_A Resolution (too) Low [sin(theta)/Lambda < 0.6]..      19.21 Deg.
PLAT031_ALERT_4_A Refined Extinction Parameter within Range .....      0.000 Sigma
PLAT245_ALERT_2_A U(iso) H3S1    Smaller than U(eq) O5S     by ...      0.320 AngSq
PLAT305_ALERT_2_A Isolated Hydrogen Atom (Outside Bond Range ??)         H3F
PLAT305_ALERT_2_A Isolated Hydrogen Atom (Outside Bond Range ??)         H4F
PLAT316_ALERT_2_A Too many H on C in C=N Moiety in Main Residue ..        C3
PLAT355_ALERT_3_A Long    O-H Bond (0.82A)   O3A    -   H3AO   ...       1.15 Ang.
PLAT417_ALERT_2_A Short Inter D-H..H-D       H1G    ..  H14A    ..       1.62 Ang.
PLAT430_ALERT_2_A Short Inter D...A Contact  O1E    ..  O2E     ..       2.37 Ang.
PLAT430_ALERT_2_A Short Inter D...A Contact  O2B    ..  O2B     ..       2.42 Ang.
PLAT430_ALERT_2_A Short Inter D...A Contact  O2D    ..  O2D     ..       2.33 Ang.
PLAT721_ALERT_1_A Bond    Calc     0.84000, Rep     0.91370 Dev...       0.07 Ang.
             O2G  -H2G     1.555   1.555                   #        113
PLAT722_ALERT_1_A Angle   Calc      109.00, Rep      117.00 Dev...       8.00 Deg.
             P1G  -O2G  -H2G     1.555   1.555   1.555      #        194
```

Alert level B

```
DIFMN02_ALERT_2_B  The minimum difference density is < -0.1*ZMAX*1.00
           _refine_diff_density_min given =     -1.680
           Test value =     -1.600
DIFMX01_ALERT_2_B  The maximum difference density is > 0.1*ZMAX*1.00
           _refine_diff_density_max given =      1.868
           Test value =      1.600
REFNR01_ALERT_3_B  Ratio of reflections to parameters is < 8 for a
           centrosymmetric structure
           sine(theta)/lambda                0.4629
           Proportion of unique data used    1.0000
           Ratio reflections to parameters   6.0182
RFACG01_ALERT_3_B  The value of the R factor is > 0.15
           R factor given   0.151
RFACR01_ALERT_3_B  The value of the weighted R factor is > 0.35
           Weighted R factor given   0.409
PLAT084_ALERT_2_B High wR2 Value ................................      0.41
PLAT088_ALERT_3_B Poor Data / Parameter Ratio ...................      6.02
PLAT097_ALERT_2_B Large Reported Max.  (Positive) Residual Density      1.87 eA-3
PLAT098_ALERT_2_B Large Reported Min.  (Negative) Residual Density     -1.68 eA-3
PLAT212_ALERT_2_B ADP of Atom O5S     is N.P.D. or (nearly) 2D ...         ?
PLAT212_ALERT_2_B ADP of Atom O1S     is N.P.D. or (nearly) 2D ...         ?
PLAT220_ALERT_2_B Large Non-Solvent    C     Ueq(max)/Ueq(min) ...       4.7 Ratio
PLAT241_ALERT_2_B Check High      Ueq as Compared to Neighbors for        C3
PLAT340_ALERT_3_B Low Bond Precision on  C-C Bonds ..............    0.0293 Ang
PLAT415_ALERT_2_B Short Inter D-H..H-X       H2B    ..  H2G     ..      2.06 Ang.
PLAT417_ALERT_2_B Short Inter D-H..H-D       H1G    ..  H3EO    ..      1.92 Ang.
PLAT420_ALERT_2_B D-H Without Acceptor      >O1G    -  >H1G    ...         ?
PLAT420_ALERT_2_B D-H Without Acceptor      <O4F    -   H4F    ...         ?
PLAT420_ALERT_2_B D-H Without Acceptor       O3D    -   H3DO   ...         ?
PLAT420_ALERT_2_B D-H Without Acceptor      *O2S    -   H1S2   ...         ?
PLAT420_ALERT_2_B D-H Without Acceptor      *O5S    -   H3S1   ...         ?
PLAT430_ALERT_2_B Short Inter D...A Contact  O1B    ..  O1D     ..      2.61 Ang.
PLAT480_ALERT_4_B Long H...A H-Bond Reported H1SB   ..  O2C     ..      3.05 Ang.
```

Alert level C

```
DIFMN03_ALERT_1_C  The minimum difference density is < -0.1*ZMAX*0.75
           The relevant atom site should be identified.
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
           The relevant atom site should be identified.
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ          ?
PLAT082_ALERT_2_C High R1 Value .................................      0.15
```

```
PLAT220_ALERT_2_C Large Non-Solvent    N     Ueq(max)/Ueq(min) ...        3.6 Ratio
PLAT222_ALERT_3_C Large Non-Solvent    H    Uiso(max)/Uiso(min) ..        4.7 Ratio
PLAT223_ALERT_4_C Large Solvent/Anion  H     Ueq(max)/Ueq(min) ...        3.1 Ratio
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for        C26
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for         N1
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for         C2
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of         P1A
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of         P1B
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of         P1C
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of         P1D
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of         P1E
PLAT245_ALERT_2_C U(iso) H1S2    Smaller than U(eq) O2S     by ...      0.044 AngSq
PLAT303_ALERT_2_C Full Occupancy H-Atom  H3CO   with # Connections       2.00
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C2     -   C3     ...       1.39 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C25    -   C26    ...       1.43 Ang.
PLAT395_ALERT_2_C Deviating  X-O-Y  Angle from 120 Deg for    *O2S      143.3 Deg.
PLAT417_ALERT_2_C Short Inter D-H..H-D       H4BO   ..  H4A     ..       2.13 Ang.
PLAT417_ALERT_2_C Short Inter D-H..H-D       H3F    ..  H3EO    ..       2.12 Ang.
PLAT420_ALERT_2_C D-H Without Acceptor       N1     -   H1B    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N11    -   H11A   ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N24    -   H24B   ...          ?
PLAT480_ALERT_4_C Long H...A H-Bond Reported H3CO   ..  S2      ..       2.96 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H1SA   ..  S1      ..       2.93 Ang.
PLAT482_ALERT_4_C Small D-H..A Angle Rep for O1S    ..  O2C     ..      99.20 Deg.
```

Alert level G

```
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: check formula stoichiometry or atom site occupancies.
          From the CIF: _cell_formula_units_Z    8
          From the CIF: _chemical_formula_sum  C20 H58.51 N6 O26 P6 S2
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C        160.00    160.00    0.00
          H        468.08    468.10   -0.02
          N         48.00     48.00    0.00
          O        208.00    207.95    0.05
          P         48.00     48.00    0.00
          S         16.00     16.00    0.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         9
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained Atom Sites ....        63
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ....         ?
PLAT007_ALERT_5_G Note: Number of Unrefined D-H Atoms .............       30
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.      0.18
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.    240.00
PLAT302_ALERT_4_G Note: Anion/Solvent Disorder ....................       20 Perc.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O2G    ..  C26     ..      2.98 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O4E    ..  C3      ..      2.98 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........       15
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #       159
              O3C  -P1C  -H3CO    1.555   1.555   1.555            28.80 Deg.
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......       293
```

```
  14 ALERT level A = Most likely a serious problem - resolve or explain
  23 ALERT level B = A potentially serious problem, consider carefully
  28 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

   7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
```

```
 46 ALERT type 2 Indicator that the structure model may be wrong or deficient
 10 ALERT type 3 Indicator that the structure quality may be low
 14 ALERT type 4 Improvement, methodology, query or suggestion
  2 ALERT type 5 Informative message, check
```

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checkCIF publication errors

Alert level A

```
PUBL006_ALERT_1_A  _publ_requested_journal is missing
            e.g. 'Acta Crystallographica Section C'
PUBL008_ALERT_1_A  _publ_section_title is missing. Title of paper.
PUBL012_ALERT_1_A  _publ_section_abstract is missing.
            Abstract of paper in English.
```

Alert level G

```
PUBL013_ALERT_1_G The _publ_section_comment (discussion of study) is
            missing. This is required for a full paper submission (but is
            optional for an electronic paper).
PUBL017_ALERT_1_G The _publ_section_references section is missing or
            empty.
```

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   3 **ALERT level A** = Data missing that is essential or data in wrong format
   2 **ALERT level G** = General alerts. Data that may be required is missing

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Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in Acta Crystallographica Section C or Section E, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. Your explanation will be considered as part of the review process.

If you intend to submit to another section of Acta Crystallographica or Journal of Applied Crystallography or Journal of Synchrotron Radiation, you should make sure that at least a basic structural check is run on the final version of your CIF prior to submission.

```
# start Validation Reply Form
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
_vrf_THETM01_I
;
PROBLEM: The value of sine(theta_max)/wavelength is less than 0.550
RESPONSE: ...
;
_vrf_PLAT023_I
;
PROBLEM: Resolution (too) Low [sin(theta)/Lambda < 0.6]..      19.21 Deg.
RESPONSE: ...
;
_vrf_PLAT031_I
;
PROBLEM: Refined Extinction Parameter within Range ......      0.000 Sigma
RESPONSE: ...
;
_vrf_PLAT245_I
;
PROBLEM: U(iso) H3S1    Smaller than U(eq) O5S     by ...      0.320 AngSq
RESPONSE: ...
;
_vrf_PLAT305_I
;
PROBLEM: Isolated Hydrogen Atom (Outside Bond Range ??)          H3F
RESPONSE: ...
;
_vrf_PLAT316_I
;
PROBLEM: Too many H on C in C=N Moiety in Main Residue ..         C3
RESPONSE: ...
;
_vrf_PLAT355_I
;
PROBLEM: Long    O-H Bond (0.82A)   O3A    -   H3AO   ...       1.15 Ang.
RESPONSE: ...
;
_vrf_PLAT417_I
;
PROBLEM: Short Inter D-H..H-D       H1G    ..  H14A    ..       1.62 Ang.
RESPONSE: ...
;
_vrf_PLAT430_I
;
PROBLEM: Short Inter D...A Contact  O1E    ..  O2E     ..       2.37 Ang.
RESPONSE: ...
;
_vrf_PLAT721_I
```

```
;
PROBLEM: Bond    Calc     0.84000, Rep     0.91370 Dev...       0.07 Ang.
RESPONSE: ...
;
_vrf_PLAT722_I
;
PROBLEM: Angle   Calc      109.00, Rep      117.00 Dev...       8.00 Deg.
RESPONSE: ...
;
# end Validation Reply Form
```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 21/12/2011; check.def file version of 16/12/2011

Datablock I - ellipsoid plot