checkCIF/PLATON report

Structure factors have been supplied for datablock(s) adnh2

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: adnh2

```
Bond precision:  C-C = 0.0113 A          Wavelength=0.71073

Cell:            a=8.5681(2)    b=39.1432(9)       c=15.1808(3)
                 alpha=90       beta=95.922(1)     gamma=90
Temperature:     293 K
```

	Calculated	Reported
Volume	5064.21(19)	5064.21(19)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C21 H32 B3 Ru2 S2, C21 H37 B3 Ru2 S2	?
Sum formula	C42 H69 B6 Ru4 S4	C21 H37 B3 Ru2 S2
Mr	1171.35	588.19
Dx,g cm-3	1.536	1.543
Z	4	8
Mu (mm-1)	1.363	1.363
F000	2364.0	2384.0
F000’	2346.22	
h,k,lmax	10,46,17	10,46,17
Nref	8646	8596
Tmin,Tmax	0.849,0.873	0.651,0.910
Tmin’	0.761	

```
Correction method= # Reported T Limits: Tmin=0.651 Tmax=0.910
AbsCorr = MULTI-SCAN

Data completeness= 0.994          Theta(max)= 24.737

R(reflections)= 0.0420( 5982)     wR2(reflections)= 0.1018( 8596)

S = 1.016                 Npar= 580
```

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

```
THETM01_ALERT_3_C  The value of sine(theta_max)/wavelength is less than 0.590
          Calculated sin(theta_max)/wavelength =    0.5888
PLAT018_ALERT_1_C _diffrn_measured_fraction_theta_max .NE. *_full          ! Check
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..       5.03 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT213_ALERT_2_C Atom C36            has ADP max/min Ratio .....        3.1 prolat
PLAT213_ALERT_2_C Atom C37            has ADP max/min Ratio .....        3.2 prolat
PLAT213_ALERT_2_C Atom C42            has ADP max/min Ratio .....        3.7 prolat
PLAT213_ALERT_2_C Atom C7             has ADP max/min Ratio .....        3.5 prolat
PLAT220_ALERT_2_C Non-Solvent  Resd 1  C   Ueq(max)/Ueq(min) Range       4.6 Ratio
PLAT220_ALERT_2_C Non-Solvent  Resd 2  C   Ueq(max)/Ueq(min) Range       3.9 Ratio
PLAT222_ALERT_3_C Non-Solv.  Resd 1  H   Uiso(max)/Uiso(min) Range       4.1 Ratio
PLAT222_ALERT_3_C Non-Solv.  Resd 2  H   Uiso(max)/Uiso(min) Range       6.0 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference Ru3      --B5       .      0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C33      --C37      .      0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C35      --C36      .      0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C37      --C38      .      0.20 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        S2 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       Ru3 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       Ru4 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C25 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C26 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C33 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C34 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C35 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C36 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       Ru2 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       RU3     0.110 Check
PLAT303_ALERT_2_C Full Occupancy Atom H21       with # Connections      2.00 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............   0.01132 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     2.462 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.589        51 Report
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.         0 Info
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Alert level G

```
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C21 H37 B3 Ru2 S2
           Atom count from the _atom_site data:  C21 H34.5 B3 Ru2 S2
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
          From the CIF: _cell_formula_units_Z    8
          From the CIF: _chemical_formula_sum  C21 H37 B3 Ru2 S2
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C         168.00    168.00    0.00
          H         296.00    276.00   20.00
          B          24.00     24.00    0.00
          Ru         16.00     16.00    0.00
          S          16.00     16.00    0.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         12 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         32 Report
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PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...       0.50 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       6.09 Why ?
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          4 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          2 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        21% Note
PLAT303_ALERT_2_G Full Occupancy Atom H2        with # Connections       2.00 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C29 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C30 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C31 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C39 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C40 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C41 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C38 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....         C7 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....         C8 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C10 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....         C6 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C18 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C19 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C20 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C16 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        259 Check
              B2   -B1   -H21     1.555   1.555   1.555            39.00 Deg.
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       196 Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        35% 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
  33 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  31 ALERT level G = General information/check it is not something unexpected

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

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_THETM01_adnh2
;
PROBLEM: The value of sine(theta_max)/wavelength is less than 0.590
RESPONSE: ...
;
_vrf_PLAT018_adnh2
;
PROBLEM: _diffrn_measured_fraction_theta_max .NE. *_full          ! Check
RESPONSE: ...
;
_vrf_PLAT041_adnh2
;
PROBLEM: Calc. and Reported SumFormula    Strings  Differ     Please Check
RESPONSE: ...
;
```

```
_vrf_PLAT043_adnh2
;
PROBLEM: Calculated and Reported Mol. Weight Differ by ..       5.03 Check
RESPONSE: ...
;
_vrf_PLAT068_adnh2
;
PROBLEM: Reported F000 Differs from Calcd (or Missing)...     Please Check
RESPONSE: ...
;
_vrf_PLAT213_adnh2
;
PROBLEM: Atom C36             has ADP max/min Ratio .....        3.1 prolat
RESPONSE: ...
;
_vrf_PLAT220_adnh2
;
PROBLEM: Non-Solvent  Resd 1  C   Ueq(max)/Ueq(min) Range        4.6 Ratio
RESPONSE: ...
;
_vrf_PLAT222_adnh2
;
PROBLEM: Non-Solv.  Resd 1  H   Uiso(max)/Uiso(min) Range        4.1 Ratio
RESPONSE: ...
;
_vrf_PLAT234_adnh2
;
PROBLEM: Large Hirshfeld Difference Ru3      --B5       .       0.16 Ang.
RESPONSE: ...
;
_vrf_PLAT241_adnh2
;
PROBLEM: High   'MainMol' Ueq as Compared to Neighbors of         S2 Check
RESPONSE: ...
;
_vrf_PLAT242_adnh2
;
PROBLEM: Low    'MainMol' Ueq as Compared to Neighbors of        Ru3 Check
RESPONSE: ...
;
_vrf_PLAT260_adnh2
;
PROBLEM: Large Average Ueq of Residue Including       RU3      0.110 Check
RESPONSE: ...
;
_vrf_PLAT303_adnh2
;
PROBLEM: Full Occupancy Atom H21       with # Connections       2.00 Check
RESPONSE: ...
;
_vrf_PLAT342_adnh2
;
PROBLEM: Low Bond Precision on  C-C Bonds ..............    0.01132 Ang.
RESPONSE: ...
;
_vrf_PLAT906_adnh2
;
PROBLEM: Large K Value in the Analysis of Variance ......      2.462 Check
RESPONSE: ...
;
_vrf_PLAT911_adnh2
;
```

```
PROBLEM: Missing FCF Refl Between Thmin & STh/L=    0.589         51 Report
RESPONSE: ...
;
_vrf_PLAT978_adnh2
;
PROBLEM: Number C-C Bonds with Positive Residual Density.          0 Info
RESPONSE: ...
;
# end Validation Reply Form
```

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* or *IUCrData*, 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 19/10/2018; check.def file version of 15/10/2018

Datablock adnh2 - ellipsoid plot