checkCIF/PLATON report

Structure factors have been supplied for datablock(s) A1

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: A1

Bond precision: C-C = 0.0203 A Wavelength=0.71073

Cell: a=16.0557(11) b=20.7694(15) c=21.3136(14)
alpha=115.639(5) beta=98.267(5) gamma=101.194(6)
Temperature: 203 K

	Calculated	Reported
Volume	6073.6(8)	6073.6(8)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C100 H88 N4 O8 Ru4, 4(C F3 O3 S), 4(C3 H6 O)	C100 H88 N4 O12 Ru4, 4 C F3 S O3, 4 C3 H6 O
Sum formula	C116 H112 F12 N4 O24 Ru4 S4	C116 H112 F12 N4 O24 Ru4 S4
Mr	2706.62	2706.61
Dx,g cm-3	1.480	1.480
Z	2	2
Mu (mm-1)	0.644	0.644
F000	2752.0	2752.0
F000’	2744.34	
h,k,lmax	22,28,29	22,28,29
Nref	33302	32944
Tmin,Tmax	0.870,0.914	
Tmin’	0.851	

Correction method= Not given

Data completeness= 0.989 Theta(max)= 29.328

R(reflections)= 0.0911(9666) wR2(reflections)= 0.2939(32944)

S = 0.836 Npar= 1113

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

SHFSU01_ALERT_2_A The absolute value of parameter shift to su ratio > 0.20
Absolute value of the parameter shift to su ratio given 0.983
Additional refinement cycles may be required.

PLAT026_ALERT_3_A	Ratio Observed / Unique Reflections (too) Low ..		29%	Check
PLAT080_ALERT_2_A	Maximum Shift/Error		0.98	Why ?
PLAT234_ALERT_4_A	Large Hirshfeld Difference C83	--C84	0.32	Ang.
PLAT234_ALERT_4_A	Large Hirshfeld Difference F4	--C102	0.32	Ang.
PLAT413_ALERT_2_A	Short Inter XH3 .. XHn H10J	..H11H	1.86	Ang.
PLAT602_ALERT_2_A	VERY LARGE Solvent Accessible VOID(S) in Structure		!	Info

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Alert level B

PLAT230_ALERT_2_B	Hirshfeld Test Diff for C97	--C99 .	8.7	s.u.
PLAT234_ALERT_4_B	Large Hirshfeld Difference S1	--C101	0.30	Ang.
PLAT234_ALERT_4_B	Large Hirshfeld Difference F5	--C102	0.26	Ang.
PLAT234_ALERT_4_B	Large Hirshfeld Difference F7	--C103	0.28	Ang.
PLAT234_ALERT_4_B	Large Hirshfeld Difference F10	--C104	0.28	Ang.
PLAT234_ALERT_4_B	Large Hirshfeld Difference F12	--C104	0.26	Ang.
PLAT241_ALERT_2_B	High 'MainMol' Ueq as Compared to Neighbors of		C83	Check
PLAT342_ALERT_3_B	Low Bond Precision on C-C Bonds		0.02026	Ang.
PLAT413_ALERT_2_B	Short Inter XH3 .. XHn H10K	..H11H	1.99	Ang.
PLAT413_ALERT_2_B	Short Inter XH3 .. XHn H10L	..H11H	1.96	Ang.

Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.150

PLAT020_ALERT_3_C	The Value of Rint is Greater Than 0.12		0.150	Report
PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)		0.29	Report
PLAT213_ALERT_2_C	Atom C83 has ADP max/min Ratio		3.9	prolat
PLAT213_ALERT_2_C	Atom C96 has ADP max/min Ratio		3.8	prolat
PLAT220_ALERT_2_C	Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range		5.2	Ratio
PLAT222_ALERT_3_C	Non-Solv. Resd 1 H Uiso(max)/Uiso(min) Range		5.9	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C67	--C68 .	6.9	s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C71	--C77 .	6.5	s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C77	--C79 .	5.3	s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C87	--C89 .	5.7	s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C97	--C98 .	5.1	s.u.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C12	--C13	0.18	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C61	--C66	0.18	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C63	--C64	0.21	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C67	--C69	0.19	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C81	--C87	0.17	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C82	--C83	0.24	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C93	--C94	0.16	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C95	--C96	0.21	Ang.
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		Ru1	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		C67	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		C87	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		C97	Check
PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of		C101	Check
PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of		C102	Check
PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of		C103	Check
PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of		C104	Check

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PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of         S1 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of         S2 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of         S3 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of         S4 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of       C105 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of       C108 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of       C111 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of       C114 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.8 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.9 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.8 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.9 Note
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C67      - C69      .       1.37 Ang.
PLAT434_ALERT_2_C Short Inter HL..HL Contact F8       ..F10             2.50 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          1 Note
            C100 H88 N4 O8 Ru4
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     81.107 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     12.950 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      4.678 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.454 Check
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.43A   From O11           -0.71 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.66A   From O20           -0.69 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  1.06A   From O21           -0.62 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.          0 Info
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Alert level G

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FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and _chemical_formula_moiety. This is
           usually due to the moiety formula being in the wrong format.
           Atom count from _chemical_formula_sum:   C116 H112 F12 N4 O24 Ru4 S4
           Atom count from _chemical_formula_moiety:C116 H112 F12 N4 O28 Ru4 S4
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.14 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          8 Report
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)  S1       --O10       .        5.6 s.u.
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)  S1       --O11       .       14.6 s.u.
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)  F3       --C101      .        8.0 s.u.
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)  S2       --O12       .       10.5 s.u.
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)  S2       --O13       .        5.2 s.u.
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)  S2       --O14       .       12.0 s.u.
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)  S2       --C102      .        8.0 s.u.
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)  F6       --C102      .        5.5 s.u.
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)  S3       --O15       .       14.7 s.u.
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)  S3       --O17       .        9.8 s.u.
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)  S3       --C103      .        7.5 s.u.
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)  S4       --O18       .       11.3 s.u.
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)  S4       --O19       .       16.3 s.u.
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)  S4       --O20       .       26.3 s.u.
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)  S4       --C104      .        9.0 s.u.
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)  F11      --C104      .        5.5 s.u.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C8       - C10      .       1.43 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C19      - C26      .       1.43 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C36      - C38      .       1.41 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C39      - C40      .       1.41 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C47      - C54      .       1.41 Ang.
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....      C115 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O17      ..C3              2.83 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O17      ..C4              2.91 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O20      ..C82             3.00 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O20      ..C33             3.02 Ang.
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PLAT432_ALERT_2_G Short Inter X...Y Contact  C109     ..C113            2.94 Ang.
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         2 Note
             C F3 O3 S
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         3 Note
             C F3 O3 S
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         4 Note
             C F3 O3 S
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         5 Note
             C F3 O3 S
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         7 Note
             C3 H6 O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         8 Note
             C3 H6 O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         9 Note
             C3 H6 O
PLAT908_ALERT_2_G Max. Perc. Data with I > 2*s(I) per Res.Shell .      71.36% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).         4 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       356 Note
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  7 ALERT level A = Most likely a serious problem - resolve or explain
 10 ALERT level B = A potentially serious problem, consider carefully
 52 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

  2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 43 ALERT type 2 Indicator that the structure model may be wrong or deficient
 11 ALERT type 3 Indicator that the structure quality may be low
 54 ALERT type 4 Improvement, methodology, query or suggestion
  0 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* 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 23/04/2018; check.def file version of 23/04/2018

Datablock A1 - ellipsoid plot