

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 2036sb15\_0m

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: 2036sb15\_0m

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Bond precision:    C-C = 0.0075 A                      Wavelength=0.71073

Cell:                      a=19.5843(8)              b=9.4572(4)              c=23.4404(10)  
                            alpha=90                      beta=96.134(2)              gamma=90

Temperature:              296 K

	Calculated	Reported
Volume	4316.6(3)	4316.6(3)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C41 H31 N7 Ru, 2(F6 P), C2 H3 N	?
Sum formula	C43 H34 F12 N8 P2 Ru	C43 H34 F12 N8 P2 Ru
Mr	1053.79	1053.79
Dx, g cm <sup>-3</sup>	1.622	1.622
Z	4	4
Mu (mm <sup>-1</sup> )	0.533	0.533
F000	2120.0	2120.0
F000'	2117.00	
h, k, lmax	26, 12, 31	26, 12, 31
Nref	11160	11077
Tmin, Tmax	0.852, 0.899	0.658, 0.746
Tmin'	0.808	

Correction method= # Reported T Limits: Tmin=0.658 Tmax=0.746  
AbsCorr = MULTI-SCAN

Data completeness= 0.993                      Theta(max)= 28.700

R(reflections)= 0.0653( 8339)

wR2(reflections)=  
0.2050( 11077)

S = 1.050

Npar= 572

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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.

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● **Alert level C**

PLAT244_ALERT_4_C	Low	'Solvent' Ueq as Compared to Neighbors of	C43	Check
PLAT250_ALERT_2_C	Large	U3/U1 Ratio for Average U(i,j) Tensor ....	2.3	Note
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including P1	0.117	Check
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including P2	0.155	Check
PLAT601_ALERT_2_C	Unit Cell	Contains Solvent Accessible VOIDS of .	32	Ang**3
PLAT906_ALERT_3_C	Large	K Value in the Analysis of Variance .....	2.895	Check
PLAT911_ALERT_3_C	Missing	FCF Refl Between Thmin & STh/L= 0.600	44	Report
PLAT918_ALERT_3_C	Reflection(s)	with I(obs) much Smaller I(calc) .	1	Check
PLAT971_ALERT_2_C	Check	Calcd Resid. Dens. 1.23Ang From F8	1.76	eA-3
PLAT971_ALERT_2_C	Check	Calcd Resid. Dens. 0.29Ang From F11	1.73	eA-3
PLAT971_ALERT_2_C	Check	Calcd Resid. Dens. 1.07Ang From F7	1.72	eA-3

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● **Alert level G**

PLAT002_ALERT_2_G	Number of	Distance or Angle Restraints on AtSite	4	Note
PLAT083_ALERT_2_G	SHELXL	Second Parameter in WGHT Unusually Large	6.89	Why ?
PLAT171_ALERT_4_G	The CIF-Embedded	.res File Contains EADP Records	1	Report
PLAT173_ALERT_4_G	The CIF-Embedded	.res File Contains DANG Records	3	Report
PLAT231_ALERT_4_G	Hirshfeld	Test (Solvent) P2 --F7 .	46.0	s.u.
PLAT231_ALERT_4_G	Hirshfeld	Test (Solvent) P2 --F8 .	50.7	s.u.
PLAT231_ALERT_4_G	Hirshfeld	Test (Solvent) P2 --F9 .	47.0	s.u.
PLAT231_ALERT_4_G	Hirshfeld	Test (Solvent) P2 --F10 .	50.3	s.u.
PLAT231_ALERT_4_G	Hirshfeld	Test (Solvent) P2 --F11 .	19.7	s.u.
PLAT244_ALERT_4_G	Low	'Solvent' Ueq as Compared to Neighbors of	P1	Check
PLAT244_ALERT_4_G	Low	'Solvent' Ueq as Compared to Neighbors of	P2	Check
PLAT790_ALERT_4_G	Centre of	Gravity not Within Unit Cell: Resd. #	4	Note
	C2 H3 N			
PLAT794_ALERT_5_G	Tentative	Bond Valency for Ru1 (III) .	2.89	Info
PLAT860_ALERT_3_G	Number of	Least-Squares Restraints .....	3	Note
PLAT883_ALERT_1_G	No Info/Value	for _atom_sites_solution_primary .		Please Do !
PLAT910_ALERT_3_G	Missing #	of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT912_ALERT_4_G	Missing #	of FCF Reflections Above STh/L= 0.600	38	Note
PLAT933_ALERT_2_G	Number of	HKL-OMIT Records in Embedded .res File	2	Note
PLAT941_ALERT_3_G	Average	HKL Measurement Multiplicity .....	4.0	Low
PLAT978_ALERT_2_G	Number	C-C Bonds with Positive Residual Density.	2	Info
PLAT992_ALERT_5_G	Repd &	Actual _reflns_number_gt Values Differ by	6	Check

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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  
21 **ALERT level G** = General information/check it is not something unexpected

1 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  
6 ALERT type 3 Indicator that the structure quality may be low  
12 ALERT type 4 Improvement, methodology, query or suggestion  
2 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.

