

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Ru\_3a

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: Ru\_3a

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Bond precision:	C-C = 0.0310 A	Wavelength=0.71073	
Cell:	a=11.6071 (16)	b=16.655 (2)	c=11.7541 (19)
	alpha=90	beta=113.396 (3)	gamma=90
Temperature:	294 K		
	Calculated	Reported	
Volume	2085.4 (5)	2085.4 (5)	
Space group	P 21	P 1 21 1	
Hall group	P 2yb	P 2yb	
Moiety formula	C42 H48 Cl N2 O4 Ru, F6 P	C42 H48 Cl F6 N2 O4 P Ru	
Sum formula	C42 H48 Cl F6 N2 O4 P Ru	C42 H48 Cl F6 N2 O4 P Ru	
Mr	926.31	926.31	
Dx, g cm <sup>-3</sup>	1.475	1.475	
Z	2	2	
Mu (mm <sup>-1</sup> )	0.548	0.548	
F000	952.0	952.0	
F000'	950.46		
h, k, lmax	13, 20, 14	13, 20, 14	
Nref	7650 [ 3968]	7605	
Tmin, Tmax	0.868, 0.972	0.870, 0.970	
Tmin'	0.868		

Correction method= # Reported T Limits: Tmin=0.870 Tmax=0.970  
AbsCorr = MULTI-SCAN

Data completeness= 1.92/0.99      Theta(max)= 25.370

R(reflections)= 0.0826 ( 4883)	wR2(reflections)=
S = 1.065	0.1847 ( 7605)
Npar= 524	

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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 B**

PLAT342\_ALERT\_3\_B Low Bond Precision on C-C Bonds ..... 0.03098 Ang.

**Author Response: This error is probably related to the combined effect of the highly irregular plate morphology of the crystal (absorption) as well as the presence of heavy element Ru. The structure is considered to be correct and no attempt was made to smash the error.**

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 **Alert level C**

RINTA01\_ALERT\_3\_C The value of Rint is greater than 0.12

Rint given 0.171

PLAT020_ALERT_3_C	The Value of Rint is Greater Than 0.12 .....	0.171	Report
PLAT031_ALERT_4_C	Refined Extinction Parameter Within Range of ...	3.143	Sigma
PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ		Please Check
PLAT090_ALERT_3_C	Poor Data / Parameter Ratio (Zmax > 18) .....	7.54	Note
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C34	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C37	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C65	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C31	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C41	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including P1	0.141	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	5	Report
PLAT973_ALERT_2_C	Check Calcd Positive Resid. Density on Ru1	1.13	eA-3

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 **Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	3	Note
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	?	Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	9.49	Why ?
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	1	Report
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of	P1	Check
PLAT303_ALERT_2_G	Full Occupancy Atom H2B with # Connections	2.00	Check
PLAT480_ALERT_4_G	Long H...A H-Bond Reported H47A ..CL1 .	2.93	Ang.
PLAT480_ALERT_4_G	Long H...A H-Bond Reported H67B ..CL1 .	2.92	Ang.
PLAT480_ALERT_4_G	Long H...A H-Bond Reported H2B ..F5 .	2.56	Ang.
PLAT721_ALERT_1_G	Bond Calc 0.97000, Rep 0.96000 Dev...	0.01	Ang.
	C28 -H28B 1_555 1_555 ..... #	52	Check
PLAT791_ALERT_4_G	Model has Chirality at C1 (Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C2 (Sohnke SpGr)	S	Verify
PLAT791_ALERT_4_G	Model has Chirality at C3 (Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C4 (Sohnke SpGr)	S	Verify
PLAT791_ALERT_4_G	Model has Chirality at C5 (Sohnke SpGr)	R	Verify
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	3	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	15	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info

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0	<b>ALERT level A</b>	= Most likely a serious problem - resolve or explain
1	<b>ALERT level B</b>	= A potentially serious problem, consider carefully
13	<b>ALERT level C</b>	= Check. Ensure it is not caused by an omission or oversight
18	<b>ALERT level G</b>	= General information/check it is not something unexpected
3	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
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.

