

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) FF471_0m_a_sq

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: FF471_0m_a_sq

Bond precision:	C-C = 0.0063 A	Wavelength=0.71073
Cell:	a=14.2851(6)	b=18.9090(8) c=29.8721(12)
	alpha=90	beta=97.011(2) gamma=90
Temperature:	150 K	
	Calculated	Reported
Volume	8008.6(6)	8008.6(6)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C69 H45 F18 N5 P4 Ru [+ solvent]	?
Sum formula	C69 H45 F18 N5 P4 Ru [+ solvent]	C69 H45 F18 N5 P4 Ru
Mr	1511.05	1511.05
Dx, g cm ⁻³	1.253	1.253
Z	4	4
Mu (mm ⁻¹)	0.356	0.356
F000	3040.0	3040.0
F000'	3038.45	
h,k,lmax	17,23,37	17,23,37
Nref	16513	16240
Tmin,Tmax	0.841,0.879	0.720,0.880
Tmin'	0.802	

Correction method= # Reported T Limits: Tmin=0.720 Tmax=0.880
AbsCorr = MULTI-SCAN

Data completeness= 0.983 Theta(max)= 26.450

R(reflections)= 0.0666(12710) wR2(reflections)= 0.2002(16238)

S = 1.436 Npar= 877

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

PLAT213_ALERT_2_A Atom F2	has ADP max/min Ratio	6.3 prolat
PLAT213_ALERT_2_A Atom F15	has ADP max/min Ratio	7.7 prolat



Alert level B

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min).	13 Note
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Alert level C

PLAT213_ALERT_2_C Atom F1	has ADP max/min Ratio	3.5 prolat
PLAT213_ALERT_2_C Atom F3	has ADP max/min Ratio	3.8 prolat
PLAT213_ALERT_2_C Atom F10	has ADP max/min Ratio	3.9 prolat
PLAT213_ALERT_2_C Atom F13	has ADP max/min Ratio	3.2 prolat
PLAT213_ALERT_2_C Atom F14	has ADP max/min Ratio	3.5 prolat
PLAT213_ALERT_2_C Atom F16	has ADP max/min Ratio	3.4 prolat
PLAT213_ALERT_2_C Atom F17	has ADP max/min Ratio	3.7 prolat
PLAT213_ALERT_2_C Atom F18	has ADP max/min Ratio	3.5 prolat
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range		3.4 Ratio
PLAT220_ALERT_2_C Non-Solvent Resd 1 F Ueq(max)/Ueq(min) Range		3.8 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for F3 -- C34 ..		5.2 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference F1 -- C34 ..		0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F14 -- C60 ..		0.19 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance		2.129 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600		47 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF		4 Note
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/SigmaW > 10 Outliers		1 Check
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.		0 Info



Alert level G

PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size	0.62 mm
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of	C34 Check
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of	C41 Check
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of	C48 Check
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of	C55 Check
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of	C60 Check
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of	C67 Check
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure	! Info
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed	! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600	217 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...	2 Note

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

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

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.

