checkCIF/PLATON report

Structure factors have been supplied for datablock(s) FF401_2_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: FF401_2_0m_a_sq

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Bond precision:  C-C = 0.0111 A          Wavelength=0.71073

Cell:            a=21.594(3)     b=27.753(4)         c=23.938(3)
                 alpha=90        beta=93.631(3)      gamma=90
Temperature:     150 K
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	Calculated	Reported
Volume	14317(3)	14317(3)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C69 H45 Cl2 F18 N3 P4 Ru [+ solvent]	?
Sum formula	C69 H45 Cl2 F18 N3 P4 Ru [+ solvent]	C69 H45 Cl2 F18 N3 P4 Ru
Mr	1553.93	1553.93
Dx,g cm-3	1.442	1.442
Z	8	8
Mu (mm-1)	0.472	0.472
F000	6240.0	6240.0
F000’	6239.28	
h,k,lmax	25,33,28	25,33,28
Nref	12799	12332
Tmin,Tmax	0.948,0.978	0.650,0.930
Tmin’	0.914	

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Correction method= # Reported T Limits: Tmin=0.650 Tmax=0.930
AbsCorr = MULTI-SCAN

Data completeness= 0.964          Theta(max)= 25.135

R(reflections)= 0.0715( 7365)     wR2(reflections)= 0.1975( 12329)

S = 1.053                 Npar= 877
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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.

Alert level A

PLAT213_ALERT_2_A Atom F5 has ADP max/min Ratio ..... 7.0 prolat
PLAT213_ALERT_2_A Atom F8 has ADP max/min Ratio ..... 5.9 prolat
PLAT213_ALERT_2_A Atom F9 has ADP max/min Ratio ..... 6.2 prolat
PLAT213_ALERT_2_A Atom F17 has ADP max/min Ratio ..... 7.1 prolat
PLAT213_ALERT_2_A Atom F18 has ADP max/min Ratio ..... 9.3 prolat
PLAT234_ALERT_4_A Large Hirshfeld Difference F16 -- C67 .. 0.32 Ang.

Alert level B

PLAT213_ALERT_2_B Atom F7 has ADP max/min Ratio ..... 4.2 prolat
PLAT213_ALERT_2_B Atom F10 has ADP max/min Ratio ..... 4.1 prolat
PLAT213_ALERT_2_B Atom F16 has ADP max/min Ratio ..... 5.0 prolat
PLAT213_ALERT_2_B Atom C67 has ADP max/min Ratio ..... 4.6 prolat
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 13 Note

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Alert level C

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low . 0.964 Note
PLAT213_ALERT_2_C Atom F6 has ADP max/min Ratio ..... 3.1 prolat
PLAT213_ALERT_2_C Atom F12 has ADP max/min Ratio ..... 3.2 oblate
PLAT213_ALERT_2_C Atom F13 has ADP max/min Ratio ..... 3.1 prolat
PLAT213_ALERT_2_C Atom C38 has ADP max/min Ratio ..... 3.5 prolat
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 6.0 Ratio
PLAT220_ALERT_2_C Non-Solvent Resd 1 F Ueq(max)/Ueq(min) Range 4.5 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference F4 -- C39 .. 0.24 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F17 -- C67 .. 0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C38 -- C39 .. 0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C53 -- C54 .. 0.16 Ang.
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C66 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01113 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ..... 3.102 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ..... 2.197 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.598 457 Report
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Info

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Alert level G

PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C32 Check
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C39 Check
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C46 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
PLAT434_ALERT_2_G Short Inter HL..HL Contact F5 .. F8 .. 2.82 Ang.
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure ! Info
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 284 Check
C67 -F16 -F17 1.555 1.555 1.555 42.50 Deg.
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed ! Info
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 34% Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 3 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 4 Note

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6 **ALERT level A** = Most likely a serious problem - resolve or explain
5 **ALERT level B** = A potentially serious problem, consider carefully

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 17 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 13 ALERT level G = General information/check it is not something unexpected

  0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 25 ALERT type 2 Indicator that the structure model may be wrong or deficient
  8 ALERT type 3 Indicator that the structure quality may be low
  8 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 13/08/2017; check.def file version of 27/07/2017

Datablock FF401_2_0m_a_sq - ellipsoid plot