

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) deh266\_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: deh266\_sq

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Bond precision:	C-C = 0.0053 A	Wavelength=0.71073
Cell:	a=33.4946(15)	b=14.0731(7)      c=23.4674(11)
	alpha=90	beta=90      gamma=90
Temperature:	150 K	
	Calculated	Reported
Volume	11061.9(9)	11061.9(9)
Space group	P c c n	P c c n
Hall group	-P 2ab 2ac	-P 2ab 2ac
Moiety formula	C52 H40 Cl2 N2 P2 Ru, 1.186(C H2 Cl2) [+ solvent]	C52 H40 Cl2 N2 P2 Ru, 1.19(C H2 Cl2)
Sum formula	C53.19 H42.37 Cl4.37 N2 P2 Ru [+ solvent]	C53.19 H42.37 Cl4.37 N2 P2 Ru
Mr	1027.52	1027.51
Dx,g cm-3	1.234	1.234
Z	8	8
Mu (mm-1)	0.586	0.586
F000	4190.6	4191.0
F000'	4188.40	
h,k,lmax	43,18,30	43,18,30
Nref	12823	12779
Tmin,Tmax	0.926,0.960	0.687,0.746
Tmin'	0.824	

Correction method= # Reported T Limits: Tmin=0.687 Tmax=0.746  
AbsCorr = MULTI-SCAN

Data completeness= 0.997      Theta(max)= 27.580

R(reflections)= 0.0485( 9400)      wR2(reflections)= 0.1294( 12779)

S = 1.085      Npar= 589

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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

PLAT213_ALERT_2_C	Atom C44	has ADP max/min Ratio .....	3.7	prolat
PLAT220_ALERT_2_C	Non-Solvent Resd 1	C Ueq(max)/Ueq(min) Range	4.3	Ratio
PLAT241_ALERT_2_C	High 'MainMol'	Ueq as Compared to Neighbors of	C4	Check
PLAT241_ALERT_2_C	High 'MainMol'	Ueq as Compared to Neighbors of	C25	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	Cl3	0.141	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	Cl5	0.138	Check
PLAT336_ALERT_2_C	Long Bond Distance for .....	C53 -Cl4	1.912	Ang.
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).		7	Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	3	Report
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

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### ● Alert level G

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: C53.19 H42.37 Cl4.37 N2 P2 Ru  
Atom count from \_chemical\_formula\_moiety:C53.19 H42.38 Cl4.38 N2 P2 Ru

CELLZ01\_ALERT\_1\_G Difference between formula and atom\_site contents detected.  
CELLZ01\_ALERT\_1\_G ALERT: check formula stoichiometry or atom site occupancies.  
From the CIF: \_cell\_formula\_units\_Z 8  
From the CIF: \_chemical\_formula\_sum C53.19 H42.37 Cl4.37 N2 P2 Ru  
TEST: Compare cell contents of formula and atom\_site data

atom	Z*formula	cif sites	diff
C	425.52	425.49	0.03
H	338.96	338.98	-0.02
Cl	34.96	34.98	-0.02
N	16.00	16.00	0.00
P	16.00	16.00	0.00
Ru	8.00	8.00	0.00

PLAT042\_ALERT\_1\_G Calc. and Reported MoietyFormula Strings Differ Please Check  
PLAT068\_ALERT\_1\_G Reported F000 Differs from Calcd (or Missing)... Please Check  
PLAT083\_ALERT\_2\_G SHELXL Second Parameter in WGHT Unusually Large 16.63 Why ?  
PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Ru1 --P1 . 5.0 s.u.  
PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Ru1 --N2 . 5.2 s.u.  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of Cl5 Constrained at 0.3333 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of Cl6 Constrained at 0.3333 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of C54 Constrained at 0.3333 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of H54A Constrained at 0.3333 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of H54B Constrained at 0.3333 Check  
PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 2 ) 100% Note  
PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 3 ) 100% Note  
PLAT304\_ALERT\_4\_G Non-Integer Number of Atoms in ..... Resd 2 4.26 Check  
PLAT304\_ALERT\_4\_G Non-Integer Number of Atoms in ..... Resd 3 1.67 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  
PLAT883\_ALERT\_1\_G No Info/Value for \_atom\_sites\_solution\_primary . Please Do !  
PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 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 ... 3 Note

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

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
12 ALERT type 2 Indicator that the structure model may be wrong or deficient  
4 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.

