

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) deh161

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: deh161

Bond precision:	C-C = 0.0114 Å	Wavelength=0.71073
Cell:	a=13.6103(4)	b=22.5386(8) c=22.1790(7)
	alpha=90	beta=106.615(1) gamma=90
Temperature:	150 K	
	Calculated	Reported
Volume	6519.5(4)	6519.5(4)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C69 H51 N9 Ru, 2(F6 P), C6 H5 F	C69 H51 N9 Ru, C6 H5 F, 2(F6 P)
Sum formula	C75 H56 F13 N9 P2 Ru	C75 H56 F13 N9 P2 Ru
Mr	1493.30	1493.29
Dx, g cm ⁻³	1.521	1.521
Z	4	4
Mu (mm ⁻¹)	0.381	0.381
F000	3040.0	3040.0
F000'	3037.38	
h,k,lmax	16,26,26	16,26,26
Nref	11239	11163
Tmin,Tmax	0.977,0.985	0.685,0.745
Tmin'	0.941	

Correction method= # Reported T Limits: Tmin=0.685 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.993 Theta(max)= 24.811

R(reflections)= 0.0752(7459) wR2(reflections)= 0.1909(11163)

S = 1.032 Npar= 1032

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

PLAT094_ALERT_2_A Ratio of Maximum / Minimum Residual Density 8.32 Report

Author Response: This may be a partially occupied chloride anion as result of incomplet

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 1.78A From C4 3.99 eA-3

Author Response: This may be a partially occupied chloride anion as result of incomplet

Alert level B

RINTA01_ALERT_3_B The value of Rint is greater than 0.18
Rint given 0.189

Author Response: The dataset provided was collected from the most suitable crystal

PLAT020_ALERT_3_B The Value of Rint is Greater Than 0.12 0.189 Report

Author Response: The dataset provided was collected from the most suitable crystal

PLAT410_ALERT_2_B Short Intra H...H Contact H11 ..H15 . 1.87 Ang.
x,y,z = 1_555 Check

Author Response: The ligand geometry enforces this short intraligand contact

Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.

PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density	4.00 eA-3
PLAT214_ALERT_2_C Atom F3B (Anion/Solvent) ADP max/min Ratio	4.2 prolat
PLAT214_ALERT_2_C Atom F4B (Anion/Solvent) ADP max/min Ratio	4.5 prolat
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range	3.7 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of	C10 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of	C70 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor	2.5 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor	2.9 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including P1B	0.113 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including P2B	0.102 Check
PLAT334_ALERT_2_C Small Aver. Benzene C-C Dist C63 -C68	1.37 Ang.
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds	0.01142 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance	6.133 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).	9 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.590	67 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.82A From C27	2.40 eA-3

Author Response: This may be a partially occupied chloride anion as result of incomplet

PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.

0 Info

● Alert level G

PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	35.97 Why ?
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) P1A --F3A .	5.3 s.u.
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
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)	100% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 5)	100% Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 2	3.85 Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 3	4.28 Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 4	3.15 Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 5	2.72 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact F2B ..C38	2.97 Ang.
	1+x,y,z =	1_655 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact F4B ..C26	2.97 Ang.
	1/2+x,1/2-y,-1/2+z =	4_665 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact F5B ..C38	2.95 Ang.
	1+x,y,z =	1_655 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact F8B ..C61	2.84 Ang.
	x,y,z =	1_555 Check
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters	2 Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still	43% Note

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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
20 ALERT type 2 Indicator that the structure model may be wrong or deficient
7 ALERT type 3 Indicator that the structure quality may be low
11 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.

