

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) deh241

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: deh241

Bond precision: C-C = 0.0086 Å

Wavelength=0.71073

Cell: a=13.8277(6) b=14.1535(7) c=21.431(1)
 alpha=71.268(2) beta=78.496(2) gamma=76.944(2)
Temperature: 150 K

	Calculated	Reported
Volume	3832.7(3)	3832.6(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C78 H60 N3 P3 Ru, 2(F6 P) [+ solvent]	C78 H60 N3 P3 Ru, 2(F6 P)
Sum formula	C78 H60 F12 N3 P5 Ru [+ solvent]	C78 H60 F12 N3 P5 Ru
Mr	1523.21	1523.21
Dx, g cm ⁻³	1.320	1.320
Z	2	2
Mu (mm ⁻¹)	0.381	0.381
F000	1552.0	1552.0
F000'	1551.27	
h,k,lmax	18,18,27	18,18,27
Nref	17842	17778
Tmin,Tmax	0.908,0.937	0.704,0.746
Tmin'	0.869	

Correction method= # Reported T Limits: Tmin=0.704 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.996

Theta(max)= 27.632

R(reflections)= 0.0770(13034)

wR2(reflections)= 0.2327(17778)

S = 1.044

Npar= 900

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 B

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min).	11	Note
PLAT934_ALERT_3_B Number of (Iobs-Icalc)/SigmaW > 10 Outliers	2	Check

Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75 The relevant atom site should be identified.		
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density	2.33	Report
PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density	3.84	eA-3
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range	3.1	Ratio
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor	2.4	Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including P5B	0.079	Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds	0.00864	Ang.
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.	0	Info

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite	7	Note
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large	0.12	Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large	14.52	Why ?
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)	0.002	Degree
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records	2	Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records	2	Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records	2	Report
PLAT231_ALERT_4_G Hirshfeld Test (Solvent) P5B --F8B .	11.7	s.u.
PLAT231_ALERT_4_G Hirshfeld Test (Solvent) P5B --F9B .	10.3	s.u.
PLAT231_ALERT_4_G Hirshfeld Test (Solvent) P5B --F11B .	8.0	s.u.
PLAT231_ALERT_4_G Hirshfeld Test (Solvent) P5B --F12B .	14.0	s.u.
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of	P4	Check
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
PLAT304_ALERT_4_G Non-Integer Number of Atoms in Resd 3	4.08	Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in Resd 4	2.92	Check
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure	!	Info
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # F6 P	3	Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints	27	Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed	!	Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600	55	Note

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
9 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
16 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.

