

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: lem44

Bond precision:	C-C = 0.0080 A	Wavelength=0.71073	
Cell:	a=16.1858(17)	b=16.1858(17)	c=33.941(4)
	alpha=90	beta=90	gamma=120
Temperature:	110 K		
	Calculated	Reported	
Volume	7701(2)	7700.6(19)	
Space group	P 31 2 1	P 31 2 1	
Hall group	P 31 2"	P 31 2"	
Moiety formula	C50 H63.24 N4 O8 Ru S [+ solvent]	C50 H63.24 N4 O8 Ru S	
Sum formula	C50 H63.24 N4 O8 Ru S [+ solvent]	C50 H63.24 N4 O8 Ru S	
Mr	981.41	981.41	
Dx, g cm ⁻³	1.270	1.270	
Z	6	6	
Mu (mm ⁻¹)	0.399	0.399	
F000	3091.4	3091.0	
F000'	3085.82		
h,k,lmax	19,19,40	19,19,40	
Nref	9163[5100]	9141	
Tmin,Tmax	0.931,0.953	0.900,0.954	
Tmin'	0.898		

Correction method= # Reported T Limits: Tmin=0.900 Tmax=0.954
AbsCorr = MULTI-SCAN

Data completeness= 1.79/1.00 Theta(max)= 25.114

R(reflections)= 0.0376(8294) wR2(reflections)= 0.0839(9141)

S = 1.021 Npar= 568

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 C

PLAT220_ALERT_2_C	Non-Solvent	Resd 1	C	Ueq(max)/Ueq(min) Range	5.4	Ratio
PLAT220_ALERT_2_C	Non-Solvent	Resd 1	N	Ueq(max)/Ueq(min) Range	3.4	Ratio
PLAT220_ALERT_2_C	Non-Solvent	Resd 1	O	Ueq(max)/Ueq(min) Range	3.2	Ratio
PLAT222_ALERT_3_C	Non-Solv.	Resd 1	H	Uiso(max)/Uiso(min) Range	5.5	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for		C4	--C29	.	5.5 s.u.
PLAT309_ALERT_2_C	Single Bonded Oxygen (C-O > 1.3 Ang)					09 Check
PLAT420_ALERT_2_C	D-H Without Acceptor		N4	--H4	.	Please Check

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite				9	Note
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms				2	Report
PLAT012_ALERT_1_G	No			_shelx_res_checksum Found in CIF		Please Check
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range			Identical	?	Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...					Please Check
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records				5	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records				2	Report
PLAT301_ALERT_3_G	Main Residue Disorder		(Resd 1)	6%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in		 Resd 1	127.24	Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety			C26	Check
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure				131	A**3
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd)			.	1.11	Ratio
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C49			--C52	1.93	Ang.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF		 #	129	Check
	C48 -C46 -C52			1.555 1.555 1.555	43.30	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF		 #	137	Check
	C53 -C46 -C49			1.555 1.555 1.555	44.20	Deg.
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group			#	13	Check
PLAT791_ALERT_4_G	Model has Chirality at C10			(Chiral SPGR)	S	Verify
PLAT791_ALERT_4_G	Model has Chirality at C29			(Chiral SPGR)	S	Verify
PLAT860_ALERT_3_G	Number of Least-Squares Restraints			7	Note
PLAT868_ALERT_4_G	ALERTS Due to the Use of _smtbx_masks Suppressed				!	Info
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File			...	4	Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain
 0 **ALERT level B** = A potentially serious problem, consider carefully
 7 **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

3 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
 3 ALERT type 3 Indicator that the structure quality may be low
 12 ALERT type 4 Improvement, methodology, query or suggestion
 1 ALERT type 5 Informative message, check

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

start Validation Reply Form

_vrf_PLAT220_lem44

;

PROBLEM: Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 5.4 Ratio

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RESPONSE: ...
;
_vrf_PLAT222_lem44
;
PROBLEM: Non-Solv. Resd 1 H Uiso(max)/Uiso(min) Range 5.5 Ratio
RESPONSE: ...
;
_vrf_PLAT230_lem44
;
PROBLEM: Hirshfeld Test Diff for C4 --C29 . 5.5 s.u.
RESPONSE: ...
;
_vrf_PLAT309_lem44
;
PROBLEM: Single Bonded Oxygen (C-O > 1.3 Ang) ..... 09 Check
RESPONSE: ...
;
_vrf_PLAT420_lem44
;
PROBLEM: D-H Without Acceptor N4 --H4 . Please Check
RESPONSE: ...
;
# end Validation Reply Form

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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 19/10/2018; check.def file version of 15/10/2018

