

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) zajc_1

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: zajc_1

Bond precision: C-C = 0.0130 Å Wavelength=1.54184

Cell: a=9.64914(19) b=21.4978(6) c=14.5013(3)
 alpha=90 beta=90 gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	3008.08(12)	3008.07(12)
Space group	P n a 21	P n a 21
Hall group	P 2c -2n	P 2c -2n
Moiety formula	C18.48 H23.44 Cl4 N5 Na 03 Ru S, 0.52(C H3)	C19 H25 Cl4 N5 Na 03 Ru S
Sum formula	C19 H25 Cl4 N5 Na 03 Ru S	C19 H25 Cl4 N5 Na 03 Ru S
Mr	669.36	669.36
Dx, g cm-3	1.478	1.478
Z	4	4
Mu (mm-1)	8.520	8.520
F000	1348.0	1348.0
F000'	1358.58	
h, k, lmax	11, 26, 18	11, 26, 17
Nref	6018[3133]	4713
Tmin, Tmax	0.351, 0.885	0.165, 0.884
Tmin'	0.006	

Correction method= # Reported T Limits: Tmin=0.165 Tmax=0.884
AbsCorr = ANALYTICAL

Data completeness= 1.50/0.78 Theta(max)= 73.270

R(reflections)= 0.0415(4388) wR2(reflections)= 0.1113(4707)

S = 1.067 Npar= 323

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	3.5	Ratio
PLAT222_ALERT_3_C	Non-Solvent Resd 1 H Uiso(max)/Uiso(min) Range	4.5	Ratio
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.8	Note
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.013	Ang.
PLAT601_ALERT_2_C	Structure Contains Solvent Accessible VOIDS of .	95	Ang3
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L= 0.600	6	Report
PLAT915_ALERT_3_C	No Flack x Check Done: Low Friedel Pair Coverage	56	%
PLAT978_ALERT_2_C	Number C-C Bonds with Positive Residual Density.	0	Info

● Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	6	Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	2	Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please	Check
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	3	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	2	Report
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)..	7%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)..	100%	Note
PLAT432_ALERT_2_G	Short Inter X...Y Contact C3A .. C4 ..	2.69	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact C3A .. C9 ..	3.19	Ang.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	12	Note
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.19	Ratio
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C3A -- C1A .	1.82	Ang.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #	29	Check
	02 -C11 -NA1 1.555 1.555 1.555	39.50	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #	132	Check
	03 -S1 -NA1 1.555 1.555 3.545	38.60	Deg.
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	19	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	45	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	11	Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully

8 **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

1 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

6 ALERT type 3 Indicator that the structure quality may be low

8 ALERT type 4 Improvement, methodology, query or suggestion

2 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.

