

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SGGSB4

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: SGGSB4

Bond precision: C-C = 0.0144 A

Wavelength=0.71073

Cell: a=8.939(2) b=9.401(2) c=16.171(4)
 alpha=92.840(9) beta=104.628(9) gamma=113.290(9)
Temperature: 150 K

	Calculated	Reported
Volume	1190.6(5)	1190.6(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C21 H39 B4 Ru2	C21 H39 B4 Ru2
Sum formula	C21 H39 B4 Ru2	C21 H39 B4 Ru2
Mr	536.90	536.90
Dx, g cm ⁻³	1.498	1.498
Z	2	2
Mu (mm ⁻¹)	1.272	1.272
F000	546.0	546.0
F000'	541.05	
h, k, lmax	11, 12, 21	11, 12, 21
Nref	5549	5402
Tmin, Tmax	0.820, 0.938	0.718, 0.938
Tmin'	0.816	

Correction method= # Reported T Limits: Tmin=0.718 Tmax=0.938
AbsCorr = MULTI-SCAN

Data completeness= 0.974

Theta(max)= 27.641

R(reflections)= 0.0726(4237)

wR2(reflections)=
0.2384(5402)

S = 1.081

Npar= 232

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**

PLAT303_ALERT_2_C	Full Occupancy Atom H3A	with # Connections	2.00	Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds		0.0144	Ang.
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	69	Report

● **Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite		10	Note
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large		0.14	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large		8.16	Why ?
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)		0.009	Degree
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records		1	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records		1	Report
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 1)	37%	Note
PLAT303_ALERT_2_G	Full Occupancy Atom H3B	with # Connections	2.00	Check
PLAT303_ALERT_2_G	Full Occupancy Atom H4	with # Connections	2.00	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn	H10B ..H20D	1.95	Ang.
		x,y,z =	1_555	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		37.30	Deg.
	B4 -B3 -H3A	1_555 1_555 1_555	# 365	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		38.00	Deg.
	RU1 -B3 -H3B	1_555 1_555 1_555	# 369	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		37.30	Deg.
	B3 -B4 -H3A	1_555 1_555 1_555	# 384	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		37.00	Deg.
	RU2 -B4 -H4	1_555 1_555 1_555	# 389	Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms		!	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		8	Note
PLAT870_ALERT_4_G	ALERTS Related to Twinning Effects Suppressed ..		!	Info
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	78	Note
PLAT931_ALERT_5_G	CIFcalcFCF Twin Law (1 1-1)	Est.d BASF	0.35	Check
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...		16	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		1.0	Low

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
8 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.

