

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) br_sq

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: br_sq

Bond precision:	C-C = 0.0047 A	Wavelength=0.71073
Cell:	a=12.2824(4)	b=30.3634(11) c=6.8630(2)
	alpha=90	beta=100.444(2) gamma=90
Temperature:	120 K	
	Calculated	Reported
Volume	2517.05(14)	2517.05(14)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C12 H8 Br2 N2 O2 Ru, C6 F4 I2 [+ solvent]	C12 H8 Br2 N2 O2 Ru, C6 F4 I2
Sum formula	C18 H8 Br2 F4 I2 N2 O2 Ru [+ solvent]	C18 H8 Br2 F4 I2 N2 O2 Ru
Mr	874.93	874.95
Dx, g cm ⁻³	2.309	2.309
Z	4	4
Mu (mm ⁻¹)	6.297	6.297
F000	1608.0	1608.0
F000'	1597.76	
h,k,lmax	16,41,9	16,41,9
Nref	3411	3387
Tmin,Tmax	0.460,0.564	0.536,0.746
Tmin'	0.237	

Correction method= # Reported T Limits: Tmin=0.536 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.993 Theta(max)= 29.145

R(reflections)= 0.0281(3032) wR2(reflections)= 0.0607(3387)

S = 1.147 Npar= 141

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

PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.413	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	11	Report



Alert level G

PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	12.01	Why ?
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ru1 --Br1 .	7.0	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ru1 --C6 .	8.6	s.u.
PLAT432_ALERT_2_G	Short Inter X...Y Contact C9 ..C9	3.16	Ang.
	-x,y,3/2-z =	2_556	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact I1 ..Br1	3.32	Ang.
	x,y,z =	1_555	Check
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure	154	A**3
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed		! Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	2	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	11	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	1	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	3	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	3	Info

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 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
3 ALERT type 4 Improvement, methodology, query or suggestion
0 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_PLAT906_br_sq
;
PROBLEM: Large K Value in the Analysis of Variance ..... 2.413 Check
RESPONSE: ...
;
_vrf_PLAT911_br_sq
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L= 0.600 11 Report
RESPONSE: ...
;
# end Validation Reply Form
```

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.

