

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

Bond precision:	S- S = 0.0003 A	Wavelength=0.71073	
Cell:	a=5.62589 (3)	b=5.62589 (3)	c=5.62589 (3)
	alpha=90	beta=90	gamma=90
Temperature:	298 K		
	Calculated	Reported	
Volume	178.063 (3)	178.063 (3)	
Space group	P a -3	P a -3	
Hall group	-P 2ac 2ab	-P 2ac 2ab	
Moiety formula	Os2.38 Rh0.32 Ru1.30 S8	?	
Sum formula	Os2.38 Rh0.32 Ru1.30 S8	Os0.59 Rh0.08 Ru0.32 S2	
Mr	873.55	218.37	
Dx, g cm ⁻³	8.146	8.146	
Z	1	4	
Mu (mm ⁻¹)	48.001	47.908	
F000	380.5	380.0	
F000'	377.02		
h, k, lmax	11, 11, 11	11, 11, 11	
Nref	281	281	
Tmin, Tmax	0.247, 0.384	0.377, 0.524	
Tmin'	0.208		

Correction method= # Reported T Limits: Tmin=0.377 Tmax=0.524
AbsCorr = GAUSSIAN

Data completeness= 1.000 Theta (max)= 47.446

R(reflections)= 0.0087 (234)	wR2(reflections)= 0.0166 (281)
S = 1.106	Npar= 8

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

PLAT041_ALERT_1_C	Calc. and Reported SumFormula	Strings Differ	Please Check
PLAT077_ALERT_4_C	Unitcell Contains Non-integer Number of Atoms ..		Please Check

● Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.250	Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT168_ALERT_4_G	The CIF-Embedded .res File Contains EXYZ Records	1	Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	1	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of Rh	Constrained at	0.08 Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	65%	Note
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	!	Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	95.0	Degree

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
10 **ALERT level G** = General information/check it is not something unexpected

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
3 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.

PLATON version of 18/05/2022; check.def file version of 17/05/2022

