

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: ad352k_150

Bond precision:	C-C = 0.0072 A	Wavelength=0.71070	
Cell:	a=20.0098(11)	b=8.0568(4)	c=10.8367(5)
	alpha=90	beta=92.795(5)	gamma=90
Temperature:	150 K		
	Calculated	Reported	
Volume	1744.96(15)	1744.96(15)	
Space group	P 21/c	P2(1)/c	
Hall group	-P 2ybc	?	
Moiety formula	4(C10 H8 S8), F6 Re	?	
Sum formula	C40 H32 F6 Re S32	C10 H8 F1.50 Re0.25 S8	
Mr	1838.79	459.69	
Dx,g cm-3	1.750	1.750	
Z	1	4	
Mu (mm-1)	2.746	2.746	
F000	913.0	913.0	
F000'	916.18		
h,k,lmax	31,12,17	31,12,17	
Nref	7168	7158	
Tmin,Tmax	0.616,0.825	0.410,1.000	
Tmin'	0.572		

Correction method= # Reported T Limits: Tmin=0.410 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 34.070

R(reflections)= 0.0929(5337) wR2(reflections)= 0.2699(7158)

S = 1.100 Npar= 226

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**

PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)	0.27	Report
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.86	Report
PLAT221_ALERT_2_C	Solv./Anion Resd 2 F Ueq(max)/Ueq(min) Range	6.9	Ratio

● **Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	2	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	1	Report
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF		Please Do !
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.25	Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.12	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	13.85	Why ?
PLAT093_ALERT_1_G	No s.u.'s on H-positions, Refinement Reported as		mixed Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Re1	Constrained at	0.25 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F1	Constrained at	0.25 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F2	Constrained at	0.25 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F3	Constrained at	0.25 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F4	Constrained at	0.25 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F5	Constrained at	0.25 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F6	Constrained at	0.25 Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 2)	1.75	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	7	Note
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL/		2018 Note

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

2 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data
6 **ALERT type 2** Indicator that the structure model may be wrong or deficient
2 **ALERT type 3** Indicator that the structure quality may be low
10 **ALERT type 4** Improvement, methodology, query or suggestion
1 **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 18/09/2020; check.def file version of 20/08/2020

