

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) lsh-r474a

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: lsh-r474a

Bond precision: C-C = 0.0047 Å Wavelength=1.34143

Cell: a=8.1070(3) b=9.9680(3) c=12.8159(4)
 alpha=105.330(3) beta=101.878(3) gamma=94.429(3)
Temperature: 150 K

	Calculated	Reported
Volume	967.87(6)	967.87(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C18 H17 Br N5 O3 Re	C18 H17 Br N5 O3 Re
Sum formula	C18 H17 Br N5 O3 Re	C18 H17 Br N5 O3 Re
Mr	617.48	617.47
Dx, g cm ⁻³	2.119	2.119
Z	2	2
Mu (mm ⁻¹)	9.762	10.252
F000	588.0	588.0
F000'	573.95	
h, k, lmax	10, 13, 16	10, 13, 16
Nref	4680	4524
Tmin, Tmax	0.269, 0.292	0.031, 0.068
Tmin'	0.172	

Correction method= # Reported T Limits: Tmin=0.031 Tmax=0.068
AbsCorr = MULTI-SCAN

Data completeness= 0.967 Theta(max)= 62.485

R(reflections)= 0.0224(4509)	wR2(reflections)=
S = 1.105	0.0604(4524)
Npar= 321	

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 B

PLAT973_ALERT_2_B Check Calcd Positive Resid. Density on Rel 1.82 eA-3



Alert level C

PLAT051_ALERT_1_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 4.78 %
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 67 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 5 Check
PLAT925_ALERT_1_C The Reported and Calculated Rho(max) Differ by . 1.01 eA-3
PLAT926_ALERT_1_C Reported and Calculated R1 Differ by -0.0020 Check
PLAT927_ALERT_1_C Reported and Calculated wR2 Differ by -0.0038 Check
PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S . 10.24 Check



Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.003 Degree
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct. 17 Note
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 = 3 Note
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Rel --C16 5.1 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Rel --C17 6.4 s.u.
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 90 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 2 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 2.4 Low
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 3 Info
PLAT984_ALERT_1_G The C-f'= 0.0150 Deviates from the B&C-Value 0.0137 Check
PLAT984_ALERT_1_G The Br-f'= -0.9500 Deviates from the B&C-Value -0.9338 Check
PLAT984_ALERT_1_G The O-f'= 0.0410 Deviates from the B&C-Value 0.0389 Check
PLAT984_ALERT_1_G The Re-f'= -6.1250 Deviates from the B&C-Value -6.5366 Check
PLAT985_ALERT_1_G The Br-f"= 1.0410 Deviates from the B&C-Value 1.0006 Check
PLAT985_ALERT_1_G The Re-f"= 4.8870 Deviates from the B&C-Value 4.7224 Check

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

- 12 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 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
1 ALERT type 5 Informative message, check
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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.

