

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mag1601_200k

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: mag1601_200k

Bond precision: C-C = 0.0042 Å

Wavelength=1.34143

Cell: a=8.2806(13) b=10.6327(16) c=22.885(4)
 alpha=91.027(14) beta=91.663(14) gamma=89.806(13)
Temperature: 200 K

	Calculated	Reported
Volume	2013.7(6)	2013.7(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C22 H20 Br2 O2	C22 H20 Br2 O2
Sum formula	C22 H20 Br2 O2	C22 H20 Br2 O2
Mr	476.18	476.20
Dx,g cm-3	1.571	1.571
Z	4	4
Mu (mm-1)	3.443	3.586
F000	952.0	952.0
F000'	945.95	
h,k,lmax	10,13,29	10,13,28
Nref	8887	8265
Tmin,Tmax	0.513,0.699	0.266,0.953
Tmin'	0.465	

Correction method= # Reported T Limits: Tmin=0.266 Tmax=0.953
AbsCorr = MULTI-SCAN

Data completeness= 0.930

Theta(max)= 59.248

R(reflections)= 0.0380(7408)

wR2(reflections)= 0.1076(8265)

S = 1.084

Npar= 470

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

PLAT051_ALERT_1_C	Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .	3.98 %
PLAT155_ALERT_4_C	The Triclinic Unitcell is NOT Reduced	Please Do !
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	20.013 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	53 Report
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .	11 Check
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..	1 Check
PLAT939_ALERT_3_C	Large Value of Not (SHELXL) Weight Optimized S .	14.89 Check

● Alert level G

ABSMU01_ALERT_1_G	Calculation of _exptl_absorpt_correction_mu not performed for this radiation type.	
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	557 Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	3 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	4.1 Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	10 Info
PLAT984_ALERT_1_G	The C-f' = 0.0148 Deviates from the B&C-Value	0.0137 Check
PLAT984_ALERT_1_G	The Br-f' = -0.9501 Deviates from the B&C-Value	-0.9338 Check
PLAT984_ALERT_1_G	The O-f' = 0.0412 Deviates from the B&C-Value	0.0389 Check
PLAT985_ALERT_1_G	The Br-f" = 1.0411 Deviates from the B&C-Value	1.0006 Check

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

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

