

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) A202300_019

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: A202300_019

Bond precision: C-C = 0.0030 Å Wavelength=0.71073

Cell: a=7.8717(3) b=15.9248(6) c=17.0044(7)
 alpha=90 beta=90 gamma=90
Temperature: 173 K

	Calculated	Reported
Volume	2131.59(14)	2131.59(14)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C12 H18 B10 Br Cl3 O2	?
Sum formula	C12 H18 B10 Br Cl3 O2	C12 H18 B10 Br Cl3 O2
Mr	488.61	488.62
Dx,g cm-3	1.523	1.523
Z	4	4
Mu (mm-1)	2.311	2.311
F000	968.0	968.0
F000'	968.86	
h,k,lmax	10,20,22	10,20,22
Nref	4904[2792]	4855
Tmin,Tmax	0.740,0.857	0.508,0.746
Tmin'	0.497	

Correction method= # Reported T Limits: Tmin=0.508 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.74/0.99 Theta(max)= 27.515

R(reflections)= 0.0218(4579) wR2(reflections)= 0.0501(4855)

S = 1.060 Npar= 259

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

PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	22	Report
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF		7	Note
PLAT987_ALERT_1_C	The Flack x is >> 0 - Do a BASF/TWIN Refinement			Please Check

● Alert level G

PLAT033_ALERT_4_G	Flack x Value Deviates > 3.0 * sigma from Zero .	0.024	Note
PLAT164_ALERT_4_G	Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.	2	Note
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C5	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C10	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact Br20 ..Cl27	3.37	Ang.
	1/2-x,1-y,1/2+z =	2_565	Check
PLAT791_ALERT_4_G	Model has Chirality at Cl3 (Sohnke SpGr)		R Verify
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	1 Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	11	Note
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged		Please Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	7	Info

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
12 **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
3 ALERT type 3 Indicator that the structure quality may be low
4 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.

