

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: Bi- O = 0.0295 A Wavelength=0.71073

Cell: a=5.4835(3) b=5.4850(3) c=28.682(2)
 alpha=90 beta=90 gamma=90
Temperature: 295 K

	Calculated	Reported
Volume	862.67(9)	862.67(10)
Space group	P 21 c n	P 21 c n
Hall group	P -2n 2a	P -2n 2a
Moiety formula	Bi8 Nb2 O16, 2(Cl)	Bi4 Cl Nb O8
Sum formula	Bi8 Cl2 Nb2 O16	Bi4 Cl Nb O8
Mr	2184.56	1092.28
Dx,g cm-3	8.410	8.410
Z	2	4
Mu (mm-1)	82.937	82.937
F000	1816.0	1816.0
F000'	1750.05	
h,k,lmax	6,6,35	6,6,35
Nref	1757[974]	1846
Tmin,Tmax	0.014,0.190	0.289,1.000
Tmin'	0.004	

Correction method= # Reported T Limits: Tmin=0.289 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.90/1.05 Theta(max)= 26.313

R(reflections)= 0.0374(1589) wR2(reflections)= 0.1001(1846)

S = 1.038 Npar= 68

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**

PLAT034_ALERT_1_C	No Flack Parameter Given. Z > Si, NonCentro	Please Do !
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.02 Report
PLAT202_ALERT_3_C	Isotropic non-H Atoms in Anion/Solvent	1 Check
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd. # Bi8 Nb2 O16	1 Note
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.489 Check

● **Alert level G**

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2 Info
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.50 Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	14.21 Why ?
PLAT111_ALERT_2_G	ADDSYM Detects New (Pseudo) Centre of Symmetry .	85 %Fit
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem b	85 %Fit
PLAT113_ALERT_2_G	ADDSYM Suggests Possible Pseudo/New Space Group	Pbcn Check
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	1 Report
PLAT794_ALERT_5_G	Tentative Bond Valency for Bi2 (III) .	2.93 Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Bi3 (III) .	2.61 Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Nb1 (V) .	5.35 Info
PLAT870_ALERT_4_G	ALERTS Related to Twinning Effects Suppressed ..	! Info
PLAT898_ALERT_4_G	Second Reported H-M Symbol in CIF Ignored	! Check
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1 Note
PLAT931_ALERT_5_G	Found Twin Law (1-1 0) [] Est. BASF	0.53 Check
PLAT931_ALERT_5_G	Found Twin Law () [1-1 0] Est. BASF	0.53 Check

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
16 **ALERT level G** = General information/check it is not something unexpected
- 3 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
3 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
6 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.

