

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Bi6Te2O15\_Pnma

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: Bi6Te2O15\_Pnma

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Bond precision:    Bi- O = 0.0092 Å                      Wavelength=0.71073

Cell:                      a=10.5831(12)              b=22.694(3)              c=5.3843(6)  
                                alpha=90                      beta=90                      gamma=90  
Temperature:              100 K

	Calculated	Reported
Volume	1293.2(3)	1293.2(3)
Space group	P n m a	P n m a
Hall group	-P 2ac 2n	-P 2ac 2n
Moiety formula	Bi6 O15 Te2	?
Sum formula	Bi6 O15 Te2	Bi6 O15 Te2
Mr	1749.08	1749.08
Dx,g cm-3	8.984	8.984
Z	4	4
Mu (mm-1)	85.867	85.869
F000	2888.0	2888.0
F000'	2796.79	
h,k,lmax	13,28,6	13,28,6
Nref	1355	1316
Tmin,Tmax	0.023,0.076	0.028,0.139
Tmin'	0.000	

Correction method= # Reported T Limits: Tmin=0.028 Tmax=0.139  
AbsCorr = NUMERICAL

Data completeness= 0.971                      Theta(max)= 26.372

R(reflections)= 0.0364( 1038)              wR2(reflections)= 0.0791( 1316)

S = 1.079                      Npar= 110

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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.

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● **Alert level C**

PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	37	Report
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	0.71A From Bi2	2.41	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	0.71A From Bi1	1.74	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	1.95A From Bi2	1.60	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.77A From Te1	-1.70	eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.78A From O8	1.00	eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.94A From O7	0.96	eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.98A From O8	0.96	eA-3

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● **Alert level G**

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension		2	Info
PLAT019_ALERT_1_G	_diffn_measured_fraction_theta_full/*_max < 1.0		0.998	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large		44.00	Why ?
PLAT794_ALERT_5_G	Tentative Bond Valency for Bi1	(III) .	3.03	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Bi2	(III) .	3.21	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Bi3	(III) .	2.88	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Bi4	(III) .	3.11	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Te1	(VI) .	5.80	Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .			Please Do !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	2	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF ....		2	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...		39	Note

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0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
8 **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  
9 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  
1 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.

