

Datablock: mo_bgo_0m

Bond precision:	Ge- 0 = 0.0050 A	Wavelength=0.71073
Cell:	a=10.5193(1) b=10.5193(1) c=10.5193(1)	
	alpha=90 beta=90 gamma=90	
Temperature: 300 K		
	Calculated	Reported
Volume	1164.02(3)	1164.02(3)
Space group	I -4 3 d	I -4 3 d
Hall group	I -4bd 2c 3	I -4bd 2c 3
Moiety formula	Bi8 Ge6 O24	Bi4 Ge3 O12
Sum formula	Bi8 Ge6 O24	Bi4 Ge3 O12
Mr	2491.50	1245.69
Dx,g cm-3	7.109	7.108
Z	2	4
Mu (mm-1)	67.947	67.947
F000	2096.0	2096.0
F000'	2040.12	
h,k,lmax	15,15,15	15,15,15
Nref	328[187]	327
Tmin,Tmax	0.047,0.033	0.374,0.746
Tmin'	0.024	
Correction method=	# Reported T Limits: Tmin=0.374	
Tmax=0.746 AbsCorr =	MULTI-SCAN	
Data completeness=	1.75/1.00 Theta(max)= 31.411	
R(reflections)= 0.0136(324)		wR2(reflections)= 0.0322(327)
S = 1.223	Npar= 16	

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

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ	Please Check
	Calc: Bi8 Ge6 O24	
	Rep.: Bi4 Ge3 O12	

Alert level G

PLAT019_ALERT_1_G	_diffraction_measured_fraction_theta_full/*_max < 1.0	0.995 Report
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.500 Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 1)	17.42 Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	3 Note
	Bi01 Ge02 O003	
PLAT794_ALERT_5_G	Tentative Bond Valency for Bi01 (III) .	3.29 Info
PLAT898_ALERT_4_G	Second Reported H-M Symbol in CIF Ignored	! Check
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	1 Note
	0 6 6,	
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities	Please Check
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	2.068 Note
	Predicted wR2: Based on SigI**2 1.56 or SHELX Weight 2.63	

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
9 **ALERT level G** = General information/check it is not something unexpected
- 3 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data
0 **ALERT type 2** Indicator that the structure model may be wrong or deficient
1 **ALERT type 3** Indicator that the structure quality may be low
3 **ALERT type 4** Improvement, methodology, query or suggestion
3 **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

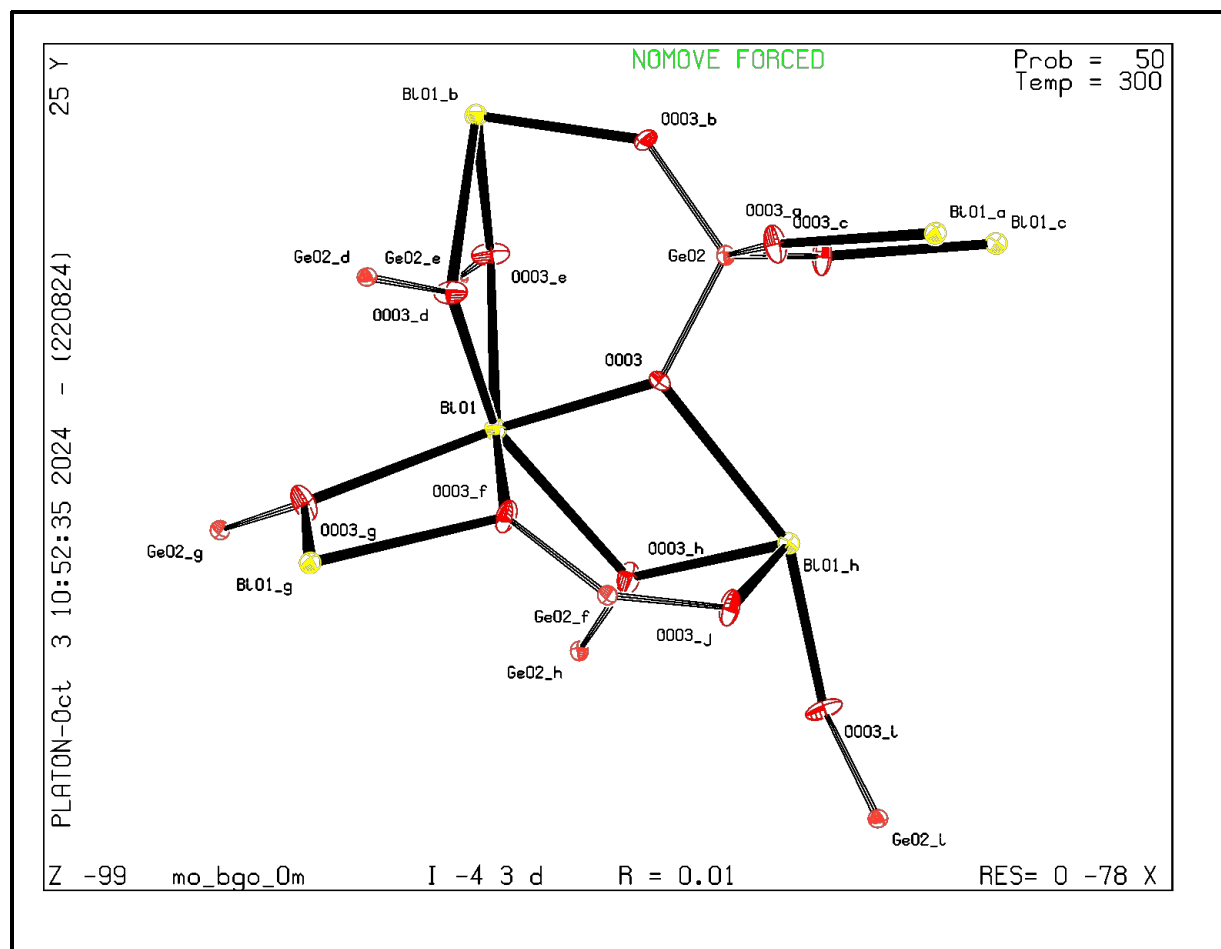
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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.

PLATON version of 22/08/2024; check.def file version of 21/08/2024

Datablock mo_bgo_0m - ellipsoid plot



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