

# Datablock: mo\_bgo\_0m

Bond precision:	Ge- 0 = 0.0050 A	Wavelength=0.71073
Cell:	a=10.5129(4)    b=10.5129(4)    c=10.5129(4)	
	alpha=90        beta=90        gamma=90	
Temperature: 220 K		
	Calculated	Reported
Volume	1161.90(13)	1161.90(13)
Space group	I -4 3 d	I -4 3 d
Hall group	I -4bd 2c 3	I -4bd 2c 3
Moiety formula	Bi8 Ge6 024	Bi4 Ge3 012
Sum formula	Bi8 Ge6 024	Bi4 Ge3 012
Mr	2491.50	1245.69
Dx,g cm-3	7.122	7.121
Z	2	4
Mu (mm-1)	68.071	68.071
F000	2096.0	2096.0
F000'	2040.12	
h,k,lmax	15,15,15	15,15,15
Nref	328[ 187]	325
Tmin,Tmax	0.047,0.033	0.376,0.746
Tmin'	0.024	
Correction method=	# Reported T Limits: Tmin=0.376	
Tmax=0.746 AbsCorr =	MULTI-SCAN	
Data completeness=	1.74/0.99    Theta(max)= 31.432	
R(reflections)= 0.0144( 323)		wR2(reflections)= 0.0344( 325)
S = 1.250	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

<a href="#">PLAT041_ALERT_1_C</a>	Calc. and Reported SumFormula    Strings   Differ	Please Check
	Calc: Bi8 Ge6 024	
	Rep.: Bi4 Ge3 012	
<a href="#">PLAT042_ALERT_1_C</a>	Calc. and Reported MoietyFormula Strings   Differ	Please Check
	Calc: Bi8 Ge6 024	
	Rep.: Bi4 Ge3 012	
<a href="#">PLAT911_ALERT_3_C</a>	Missing FCF Refl Between Thmin & STh/L=    0.600	2 Report
	0 3 5,    0 6 6,	
<a href="#">PLAT972_ALERT_2_C</a>	Check Calcd Resid. Dens.    0.76Ang From Bi01	-1.57 eA-3

## Alert level G

<a href="#">PLAT019_ALERT_1_G</a>	diffn measured fraction_theta_full/*_max < 1.0	0.992 Report
<a href="#">PLAT045_ALERT_1_G</a>	Calculated and Reported Z Differ by a Factor ...	0.500 Check
<a href="#">PLAT304_ALERT_4_G</a>	Non-Integer Number of Atoms in ..... (Resd    1)	17.42 Check
<a href="#">PLAT720_ALERT_4_G</a>	Number of Unusual/Non-Standard Labels ..... Bi01    Ge02    0003	3 Note
<a href="#">PLAT794_ALERT_5_G</a>	Tentative Bond Valency for Bi01    (III)    .	3.29 Info
<a href="#">PLAT898_ALERT_4_G</a>	Second Reported H-M Symbol in CIF Ignored .....	! Check
<a href="#">PLAT913_ALERT_3_G</a>	Missing # of Very Strong Reflections in FCF .... 0 6 6,	1 Note
<a href="#">PLAT933_ALERT_2_G</a>	Number of HKL-OMIT Records in Embedded .res File 1 1 6,	1 Note
<a href="#">PLAT961_ALERT_5_G</a>	Dataset Contains no Negative Intensities .....	Please Check
<a href="#">PLAT969_ALERT_5_G</a>	The 'Henn et al.' R-Factor-gap value ..... Predicted wR2: Based on SigI**2    1.49 or SHELX Weight    2.76	2.311 Note

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
10 **ALERT level G** = General information/check it is not something unexpected
- 4 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  
2 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.

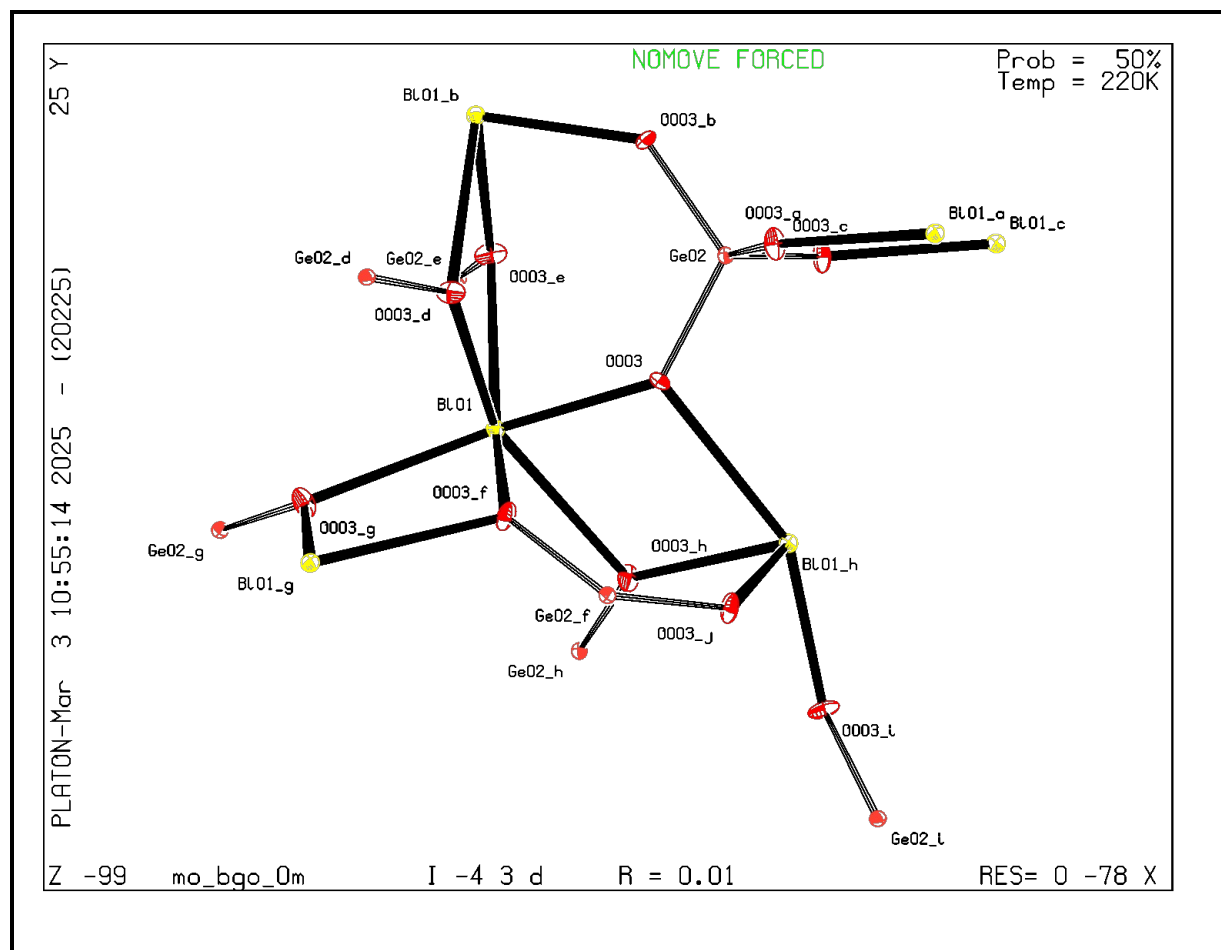
### Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

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PLATON version of 02/02/2025; check.def file version of 02/02/2025

### Datablock mo\_bgo\_0m - ellipsoid plot



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