

Datablock: mo_bgo_0m

Bond precision:	Ge- 0 = 0.0050 A	Wavelength=0.71073
Cell:	a=10.51690(12) b=10.51690(12) c=10.51690(12)	
	alpha=90 beta=90 gamma=90	
Temperature:	260 K	
	Calculated	Reported
Volume	1163.22(4)	1163.22(4)
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	7.114	7.113
Z	2	4
Mu (mm-1)	67.994	67.994
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)= 31.419	
R(reflections)= 0.0141(325)		wR2(reflections)= 0.0331(327)
S = 1.281	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				
PLAT041_ALERT_1_C	Calc. and Reported SumFormula	Strings Differ		Please Check
	Calc: Bi8 Ge6 024			
	Rep.: Bi4 Ge3 012			
PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula	Strings Differ		Please Check
	Calc: Bi8 Ge6 024			
	Rep.: Bi4 Ge3 012			
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.73Ang From Bi01		-1.65 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	0.92Ang From 0003	.	-0.43 eA-3

●Alert level G				
PLAT019_ALERT_1_G	_diffn_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
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large			6.38 Why ?
PLAT180_ALERT_4_G	Check Cell Rounding: # of Values Ending with 0 =			3 Note
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 0003			
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			2.139 Note
	Predicted wR2: Based on SigI**2 1.55 or SHELX Weight			2.59

- 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
- 11 **ALERT level G** = General information/check it is not something unexpected
- 4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
- 3 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
- 4 ALERT type 4 Improvement, methodology, query or suggestion
- 3 ALERT type 5 Informative message, check

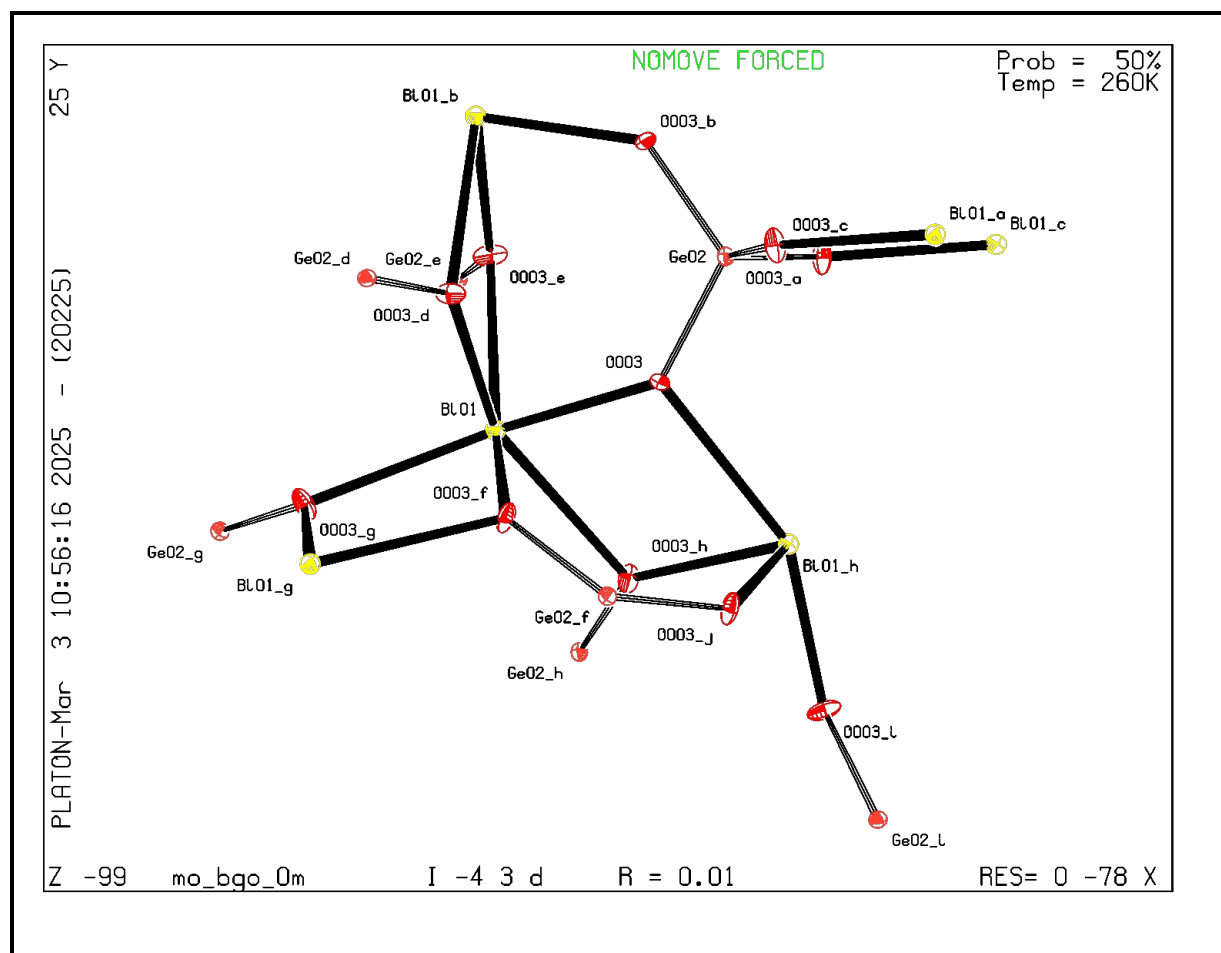
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details

Publication of your CIF in IUCr journals

Publication of your CIF in other journals

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

Datablock mo bgo 0m - ellipsoid plot



[Download CIF editor \(publCIF\) from the IUCr](#)
[Download CIF editor \(enCIFer\) from the CCDC](#)
[Test a new CIF entry](#)