

Datablock: mo_bgo_0m

| | | |
|----------------------|--|-----------------------------------|
| Bond precision: | Ge- 0 = 0.0050 A | Wavelength=0.71073 |
| Cell: | a=10.5123(3) b=10.5123(3) c=10.5123(3) | |
| | alpha=90 beta=90 gamma=90 | |
| Temperature: | 140 K | |
| | Calculated | Reported |
| Volume | 1161.70(10) | 1161.70(10) |
| 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 | 7.123 | 7.122 |
| Z | 2 | 4 |
| Mu (mm-1) | 68.083 | 68.083 |
| F000 | 2096.0 | 2096.0 |
| F000' | 2040.12 | |
| h,k,lmax | 15,15,15 | 15,15,15 |
| Nref | 328[187] | 326 |
| Tmin,Tmax | 0.047,0.033 | 0.343,0.746 |
| Tmin' | 0.024 | |
| Correction method= | # Reported T Limits: Tmin=0.343 | |
| Tmax=0.746 AbsCorr = | MULTI-SCAN | |
| Data completeness= | 1.74/0.99 Theta(max)= 31.434 | |
| R(reflections)= | 0.0146(325) | wR2(reflections)= 0.0344(326) |
| S = | 1.235 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 O24 | | |
| | Rep.: Bi4 Ge3 O12 | | |
| PLAT042_ALERT_1_C | Calc. and Reported MoietyFormula | Strings Differ | Please Check |
| | Calc: Bi8 Ge6 O24 | | |
| | Rep.: Bi4 Ge3 O12 | | |

Alert level G

| | | |
|-----------------------------------|---|--------------|
| 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 | 7.96 Why ? |
| 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) . | 3.27 Info |
| PLAT898_ALERT_4_G | Second Reported H-M Symbol in CIF Ignored | ! Check |
| PLAT933_ALERT_2_G | Number of HKL-OMIT Records in Embedded .res File | 1 Note |
| | 1 1 6, | |
| PLAT961_ALERT_5_G | Dataset Contains no Negative Intensities | Please Check |
| PLAT969_ALERT_5_G | The 'Henn et al.' R-Factor-gap value | 1.994 Note |
| | Predicted wR2: Based on SigI**2 1.73 or SHELX Weight 2.79 | |

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully

2 **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

2 **ALERT type 2** Indicator that the structure model may be wrong or deficient

0 **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

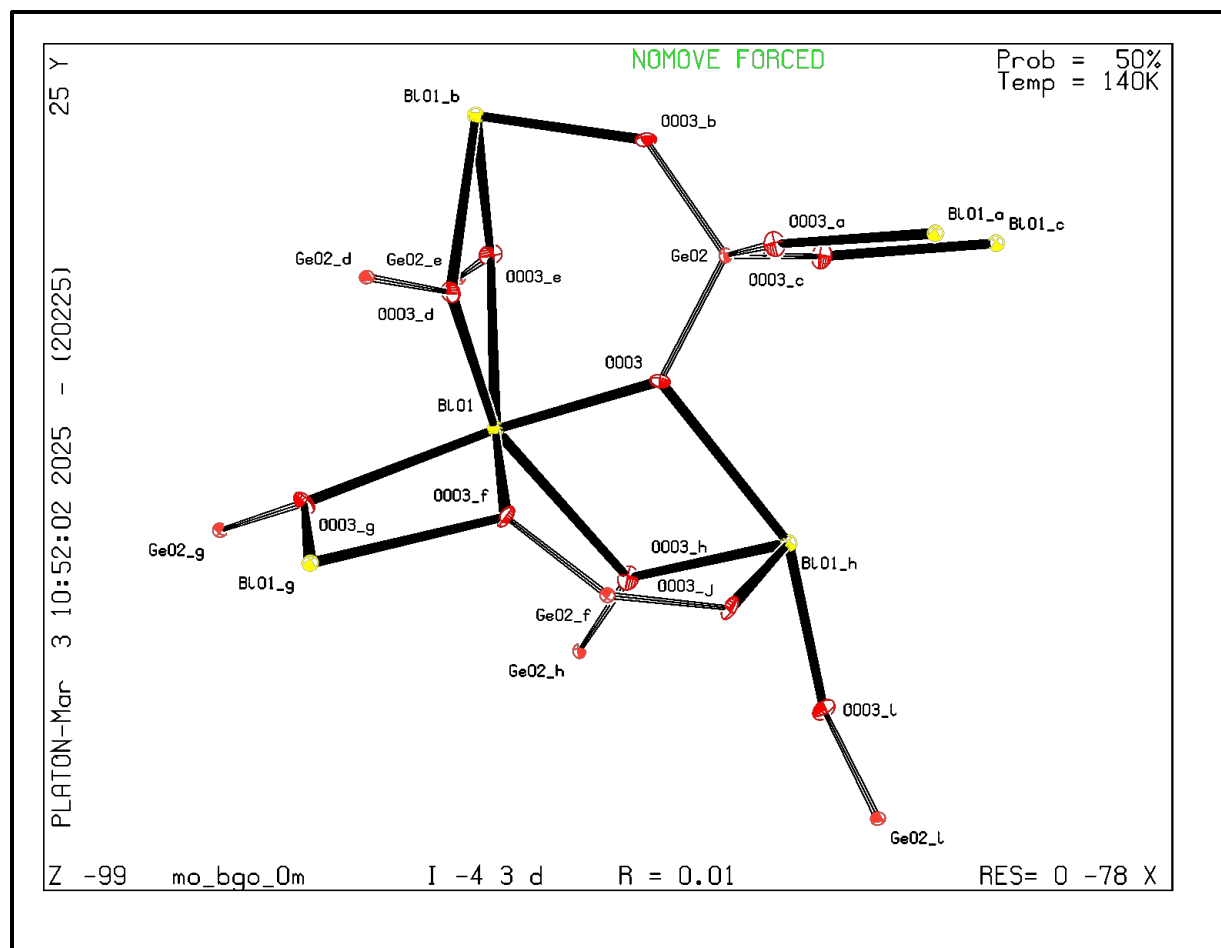
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *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 02/02/2025; check.def file version of 02/02/2025

Datablock mo_bgo_0m - ellipsoid plot



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