

checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...

Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait

```
[/usr/lib/cgi-bin/checkcif_with_hkl] cd /tmp/checkcif_hkl/_dvn47A0o5L6jd/ ;  
/Local/DataComm/submissions/platon/process_fcf.pl -sup 47A0o5L6jd.cif &
```

....

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) mo_b2262_0m

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](#)

Please wait while processing [Interpreting this report](#)

Structure factor report

Datablock: mo_b2262_0m

Bond precision:	C-C = 0.0060 Å	Wavelength=0.71073
Cell:	a=12.8215(6) b=13.5748(6) c=15.1534(8)	
	alpha=85.829(2) beta=73.537(2) gamma=68.789(2)	
Temperature: 100 K		
	Calculated	Reported
Volume	2356.7(2)	2356.7(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C32 H36 Bi2 I6 N4 O4 S4	C32 H36 Bi2 I6 N4 O4 S4
Sum formula	C32 H36 Bi2 I6 N4 O4 S4	C32 H36 Bi2 I6 N4 O4 S4
Mr	1848.25	1848.25
Dx, g cm ⁻³	2.605	2.605
Z	2	2
Mu (mm ⁻¹)	11.602	11.602
F000	1672.0	1672.0
F000'	1652.18	
h,k,lmax	18,19,21	18,19,21
Nref	14455	14441
Tmin,Tmax	0.226,0.429	0.255,0.433
Tmin'	0.161	
Correction method= # Reported T Limits: Tmin=0.255 Tmax=0.433 AbsCorr =		
MULTI-SCAN		
Data completeness= 0.999	Theta(max)= 30.560	
R(reflections)= 0.0286(12134)	WR2(reflections)= 0.0513(14441)	
S = 1.082	Npar= 489	

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

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 2 Report

●Alert level G

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 5.34 Why ?

PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.002 Degree

PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Bi1 --I3 . 13.4 s.u.

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 1 Note

PLAT794_ALERT_5_G	Tentative Bond Valency for Bi1	(III)	.	3.09	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Bi2	(III)	.	3.10	Info
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).			2	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600		11	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.			1	Info

- 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

- 1 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
 2 ALERT type 3 Indicator that the structure quality may be low
 2 ALERT type 4 Improvement, methodology, query or suggestion
 2 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

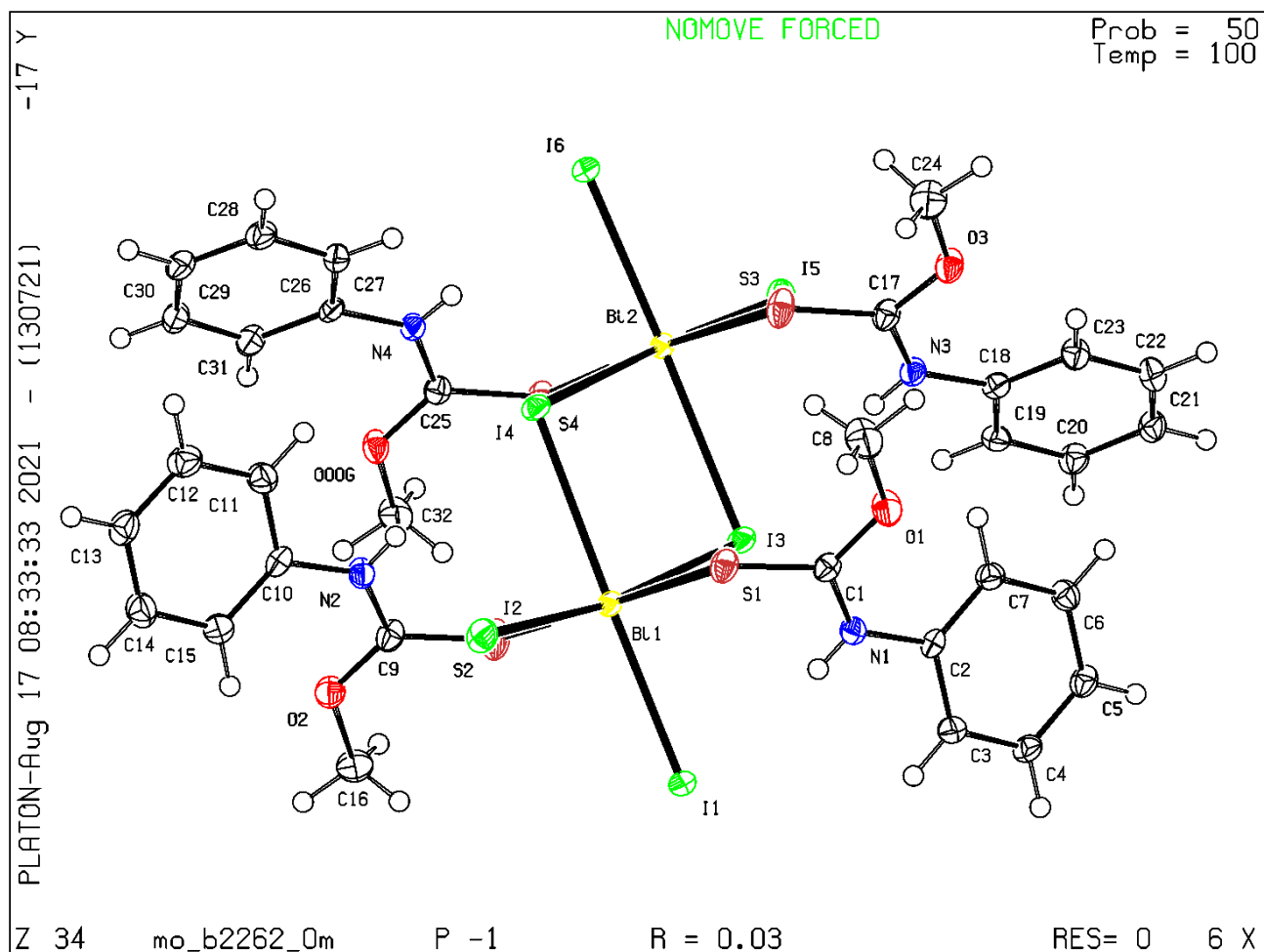
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 13/07/2021; check.def file version of 13/07/2021

Datablock mo_b2262_0m - ellipsoid plot



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