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 . . . . . .

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) CuBr-BisM

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: CuBr-BisM

Bond precision: C-C = 0.0071 A Wavelength=0.71073

Cell: a=15.7124(2) b=25.0060(3) c=36.9047(5)
alpha=90 beta=90 gamma=90

Temperature: 123 K

	Calculated	Reported
Volume	14500.0(3)	14500.0(3)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C75 H66 Br2 Cu3 P6, C4 H10 O, Br	C75 H66 Br2 Cu3 P6, Br, C4 H10 O
Sum formula	C79 H76 Br3 Cu3 O P6	C79 H76 Br3 Cu3 O P6
Mr	1657.57	1657.56
Dx,g cm-3	1.519	1.519
Z	8	8
Mu (mm-1)	2.703	2.703
F000	6720.0	6720.0
F000'	6727.40	
h,k,lmax	21,34,50	21,34,49
Nref	19517	19341
Tmin,Tmax	0.547,0.729	0.889,1.000
Tmin'	0.536	

Correction method= # Reported T Limits: Tmin=0.889 Tmax=1.000 AbsCorr = MULTI-SCAN

Data completeness= 0.991 Theta(max)= 29.130

R(reflections)= 0.0577(13921) wR2(reflections)= 0.1362(19341)

S = 1.056 Npar= 878

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: C75 H66 Br2 Cu3 P6, C4 H10 O, Br
Rep.: C75 H66 Br2 Cu3 P6, Br, C4 H10 O
PLAT260_ALERT_2_C Large Average Ueq of Residue Including O1A 0.142 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including O1B 0.117 Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00713 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 8.241 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.128 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 18 Report
2 1 0, 0 16 0, 1 2 3, 1 3 4, 0 2 6, 0 0 8,
0 0 42, 0 2 42, 1 1 43, 0 2 43, 0 4 43, 0 6 43,
0 0 44, 1 0 44, 1 1 44, 0 2 44, 1 2 44, 1 3 44,
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.36Ang From C38 1.62 eA-3

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.19Ang From Br3B 1.55 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H75 . -0.33 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H77D . -0.42 eA-3

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 10 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 8 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 28.81 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 3 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 6 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records 3 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 19 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 3 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 2 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Br1 --Cu1 . 7.0 s.u.
And 5 other PLAT232 Alerts
More ...
PLAT300_ALERT_4_G Atom Site Occupancy of O1A Constrained at 0.6 Check
And 32 other PLAT300 Alerts
More ...
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 100% Note
And 4 other PLAT302 Alerts
More ...
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 4) 0.50 Check
And 2 other PLAT304 Alerts
More ...
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O1A . 107.0 Degree
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O1B . 104.0 Degree
PLAT413_ALERT_2_G Short Inter XH3 .. XHn H13A ..H79F . 2.09 Ang.
x,y,z = 1_555 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn H59 ..H79E . 1.99 Ang.
1+x,y,z = 1_655 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact Br3B ..C24 . 3.33 Ang.
1/2-x,1/2+y,z = 8_665 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact Br3B ..C65 . 3.33 Ang.
x,y,z = 1_555 Check
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C78B --C79B 1.74 Ang.
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 114 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
0 0 2,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 144 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 5 Note
0 0 8, 0 2 6, 1 2 3, 1 3 4, 2 1 0,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 3.26 Note
Predicted wR2: Based on SigI**2 4.18 or SHELX Weight 13.21
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
11 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
72 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
24 ALERT type 2 Indicator that the structure model may be wrong or deficient
8 ALERT type 3 Indicator that the structure quality may be low
49 ALERT type 4 Improvement, methodology, query or suggestion
1 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

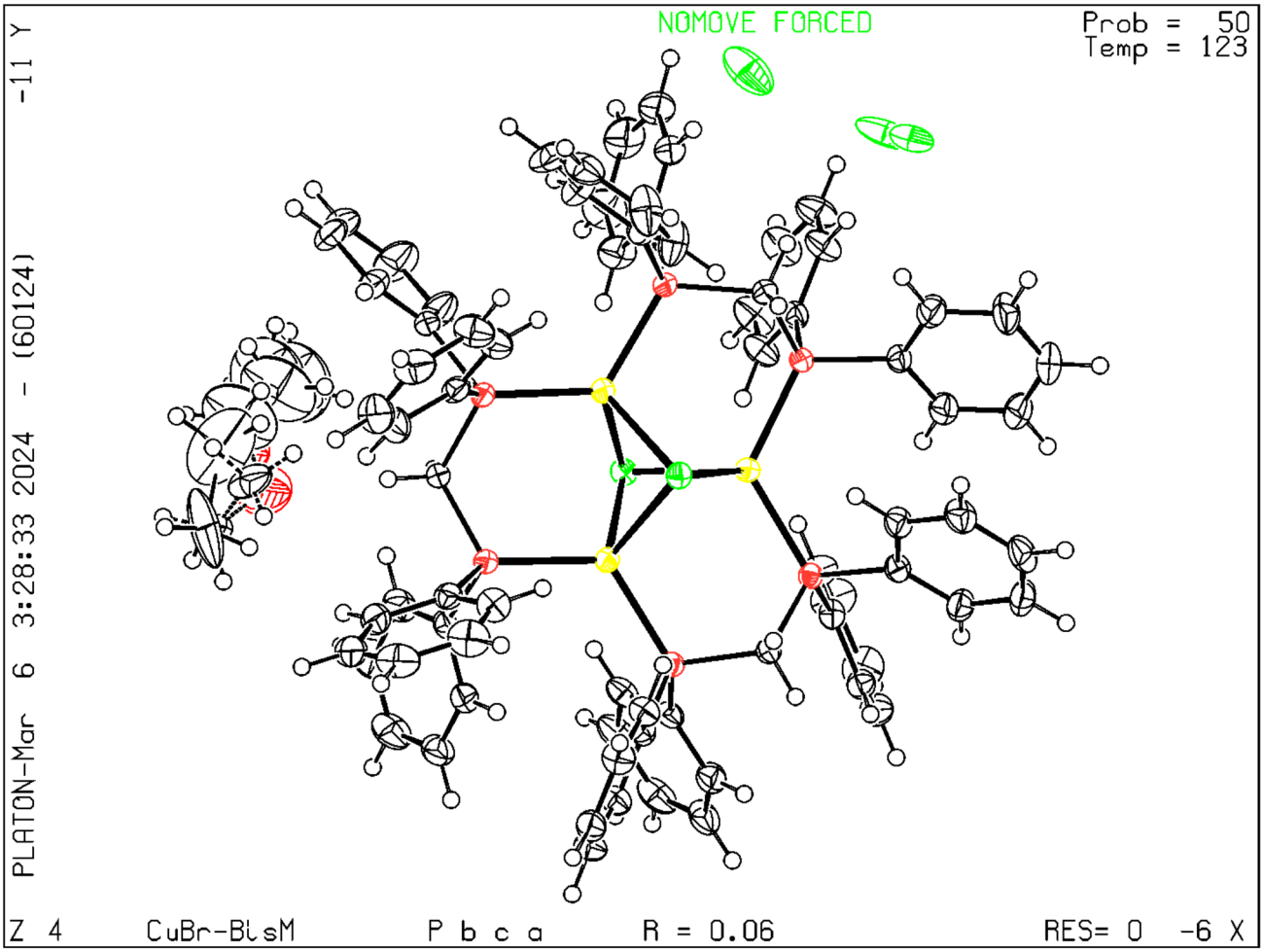
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 06/01/2024; check.def file version of 05/01/2024

Datablock CuBr-BisM - ellipsoid plot



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