

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) isn162_130k_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 Interpreting this report

Datablock: isn162_130k_0m

Bond precision: C-C = 0.0040 A

Wavelength=1.54178

Cell: a=10.1768(8) b=13.7504(11) c=20.1505(16)
 alpha=90.204(2) beta=98.120(2) gamma=99.535(2)
Temperature: 130 K

	Calculated	Reported
Volume	2751.9(4)	2751.9(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C51 H38 Br2 Cu N2 O P2, F6 P, 0.7(C4 H10 O), 1.1(C H2 P, 1.1(C H2 Cl2), 0.7(C4 Cl2)	C51 H38 Br2 Cu N2 O P2, F6 H10 O)
Sum formula	C54.90 H47.20 Br2 Cl2.20 Cu F6 N2 O1.70 P3	C54.90 H47.20 Br2 Cl2.20 Cu F6 N2 O1.70 P3
Mr	1270.40	1270.40
Dx, g cm ⁻³	1.533	1.533
Z	2	2
Mu (mm ⁻¹)	4.597	4.597
F000	1279.2	1279.0
F000'	1278.98	
h,k,lmax	12,16,24	12,16,24
Nref	10524	10241
Tmin,Tmax	0.542,0.603	0.626,0.753
Tmin'	0.416	

Correction method= # Reported T Limits: Tmin=0.626 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 0.973

Theta(max)= 70.285

R(reflections)= 0.0382(9939)

wR2(reflections)= 0.1101(10241)

S = 1.073

Npar= 728

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 B

PLAT934_ALERT_3_B Number of (Iobs-Icalc)/SigmaW > 10 Outliers 4 Check

Alert level C

PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ... 2.64 Report
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.1 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C50 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 71 Report

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 17 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 17 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.002 Degree
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 2 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 2 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 3 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 5 Report
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of P3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O2 Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C53 Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C54 Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C55 Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C56 Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H53A Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H53B Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H53C Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H54A Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H54B Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H55A Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H55B Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H56A Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H56B Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H56C Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C11 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C12 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C52 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H52A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H52B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C13 Constrained at 0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C14 Constrained at 0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C57 Constrained at 0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H57A Constrained at 0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H57B Constrained at 0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C15 Constrained at 0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C16 Constrained at 0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C59 Constrained at 0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H59A Constrained at 0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H59B Constrained at 0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C17 Constrained at 0.1 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C18 Constrained at 0.1 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C58 Constrained at 0.1 Check

PLAT300_ALERT_4_G	Atom Site Occupancy of H58A	Constrained at	0.1	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H58B	Constrained at	0.1	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 5)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 6)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 7)		100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 3		10.50	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 4		2.50	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 5		1.50	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 7		0.50	Check
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #		3	Note
	C4 H10 O			
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #		5	Note
	C H2 Cl2			
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		136	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		212	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...		1	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
 1 **ALERT level B** = A potentially serious problem, consider carefully
 5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 60 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 7 ALERT type 2 Indicator that the structure model may be wrong or deficient
 4 ALERT type 3 Indicator that the structure quality may be low
 53 ALERT type 4 Improvement, methodology, query or suggestion
 0 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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