

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cu_20221245_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: cu_20221245_0m

Bond precision: C-C = 0.0039 A Wavelength=1.54184

Cell: a=14.6382 (13) b=8.7434 (8) c=14.8811 (14)

 alpha=90 beta=112.727 (4) gamma=90

Temperature: 170 K

	Calculated	Reported
Volume	1756.7 (3)	1756.7 (3)
Space group	P 21	P 1 21 1
Hall group	P 2yb	P 2yb
Moiety formula	C23 H34 F3 N5 O5, C6 H12 O2	C23 H34 F3 N5 O5, C6 H12 O2
Sum formula	C29 H46 F3 N5 O7	C29 H46 F3 N5 O7
Mr	633.71	633.71
Dx, g cm ⁻³	1.198	1.198
Z	2	2
Mu (mm ⁻¹)	0.811	0.811
F000	676.0	676.0
F000'	678.37	
h, k, lmax	18, 10, 18	18, 10, 18
Nref	7235 [3866]	7094
Tmin, Tmax	0.885, 0.907	0.612, 0.754
Tmin'	0.885	

Correction method= # Reported T Limits: Tmin=0.612 Tmax=0.754

AbsCorr = MULTI-SCAN

Data completeness= 1.83/0.98

Theta (max)= 74.885

R(reflections)= 0.0396 (6531)

wR2(reflections)=
0.1049 (7094)

S = 1.048

Npar= 452

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

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.27	Report
PLAT234_ALERT_4_C	Large Hirshfeld Difference C50 --C52 .	0.18	Ang.

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	3	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	9	Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	5	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	1	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	2	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0100	Report
PLAT190_ALERT_3_G	A Non-default RIGU Restraint Value for First Par	0.0100	Report
PLAT190_ALERT_3_G	A Non-default RIGU Restraint Value for SecondPar	0.0200	Report
PLAT190_ALERT_3_G	A Non-default RIGU Restraint Value for First Par	0.0100	Report
PLAT190_ALERT_3_G	A Non-default RIGU Restraint Value for SecondPar	0.0200	Report
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C1	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O12 Constrained at	0.552	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O12A Constrained at	0.448	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C49 Constrained at	0.552	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C50 Constrained at	0.552	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C51 Constrained at	0.552	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C52 Constrained at	0.552	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C49A Constrained at	0.448	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C50A Constrained at	0.448	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C51A Constrained at	0.448	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C52A Constrained at	0.448	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H49A Constrained at	0.552	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H49B Constrained at	0.552	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H50 Constrained at	0.552	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H51A Constrained at	0.552	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H51B Constrained at	0.552	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H51C Constrained at	0.552	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H52A Constrained at	0.552	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H52B Constrained at	0.552	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H52C Constrained at	0.552	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H49C Constrained at	0.448	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H49D Constrained at	0.448	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H50A Constrained at	0.448	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H51D Constrained at	0.448	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H51E Constrained at	0.448	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H51F Constrained at	0.448	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H52D Constrained at	0.448	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H52E Constrained at	0.448	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H52F Constrained at	0.448	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	63%	Note
PLAT791_ALERT_4_G	Model has Chirality at C3 (Sohnke SpGr)	S	Verify
PLAT791_ALERT_4_G	Model has Chirality at C10 (Sohnke SpGr)	S	Verify
PLAT791_ALERT_4_G	Model has Chirality at C14 (Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C15 (Sohnke SpGr)	S	Verify

PLAT791_ALERT_4_G Model has Chirality at C17	(Sohnke SpGr)	S Verify
PLAT791_ALERT_4_G Model has Chirality at C20	(Sohnke SpGr)	S Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints		158 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600		20 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.		0 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by		2 Check

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
51 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 ALERT type 3 Indicator that the structure quality may be low
40 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.

