

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mfr200009

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: mfr200009

Bond precision: C-C = 0.0056 Å Wavelength=1.54184

Cell: a=14.9090(3) b=20.2337(3) c=16.0723(4)
 alpha=90 beta=94.937(2) gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	4830.45(17)	4830.45(17)
Space group	I 2/a	I 1 2/a 1
Hall group	-I 2ya	-I 2ya
Moiety formula	C32 H28 Cu2 N8 S4, 2(C2 F6 N O4 S2)	C32 H28 Cu2 N8 S4, 2(C2 F6 N O4 S2)
Sum formula	C36 H28 Cu2 F12 N10 O8 S8	C36 H28 Cu2 F12 N10 O8 S8
Mr	1340.26	1340.24
Dx, g cm ⁻³	1.843	1.843
Z	4	4
Mu (mm ⁻¹)	5.307	5.307
F000	2688.0	2688.0
F000'	2691.50	
h,k,lmax	17,24,19	17,24,19
Nref	4304	4236
Tmin,Tmax	0.431,0.727	0.669,1.000
Tmin'	0.266	

Correction method= # Reported T Limits: Tmin=0.669 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.984 Theta(max)= 66.896

R(reflections)= 0.0473(3636) wR2(reflections)= 0.1333(4236)

S = 1.039 Npar= 487

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

PLAT088_ALERT_3_C	Poor Data / Parameter Ratio	8.70	Note
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.4	Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.597	68	Report



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	34	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	32	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	9.69	Why ?
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	40	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	3	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	1	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of C15A Constrained at	0.6281	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C15B Constrained at	0.3719	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H15A Constrained at	0.6281	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H15B Constrained at	0.6281	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H16A Constrained at	0.6281	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H16B Constrained at	0.6281	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H15C Constrained at	0.3719	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H15D Constrained at	0.3719	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H16C Constrained at	0.3719	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H16D Constrained at	0.3719	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of S3 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of S4 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F1 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F2 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F3 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F4 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F5 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F6 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O1 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O2 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O3 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O4 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N5 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C17 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C18 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of S5 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of S6 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F7 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F8 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F9 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F10 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F11 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F12 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O5 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O6 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O7 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O8 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N6 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C19 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C20 Constrained at	0.5	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	4%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	100%	Note

PLAT304_ALERT_4_G Non-Integer Number of Atoms in	(Resd 2)	7.50	Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in	(Resd 3)	7.50	Check
PLAT432_ALERT_2_G Short Inter X...Y Contact F8	..C1	2.72	Ang.
	x,y,z =	1_555	Check
PLAT432_ALERT_2_G Short Inter X...Y Contact F8	..C2	2.74	Ang.
	x,y,z =	1_555	Check
PLAT432_ALERT_2_G Short Inter X...Y Contact O4	..C2	3.00	Ang.
	3/2-x,1/2-y,1/2-z =	7_655	Check
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group #		30	Check
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms		!	Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints		625	Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still		77%	Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity		4.8	Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.		0	Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
3 **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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
8 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
48 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 05/12/2020; check.def file version of 05/12/2020

Datablock mfr200009 - ellipsoid plot

