

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) zfwang13cult

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: zfwang13cult

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

Cell: a=10.0533 (3) b=12.3212 (4) c=20.8828 (6)
 alpha=81.005 (3) beta=84.188 (3) gamma=68.344 (3)
Temperature: 100 K

	Calculated	Reported
Volume	2371.90 (14)	2371.90 (14)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2 (C22 H33 I O4 S), H2 O	C22 H33 I O4 S, 0.5 (H2 O)
Sum formula	C44 H68 I2 O9 S2	C22 H34 I O4.50 S
Mr	1058.90	529.45
Dx, g cm ⁻³	1.483	1.483
Z	2	4
Mu (mm ⁻¹)	11.643	11.643
F000	1084.0	1084.0
F000'	1086.86	
h, k, lmax	12, 15, 26	12, 15, 26
Nref	10003	9599
Tmin, Tmax	0.522, 0.705	0.584, 1.000
Tmin'	0.422	

Correction method= # Reported T Limits: Tmin=0.584 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.960 Theta (max)= 76.767

R(reflections)= 0.0289 (8919)	wR2(reflections)=
S = 1.040	0.0741 (9599)
Npar= 561	

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
PLAT230_ALERT_2_C	Hirshfeld Test Diff for I1A --C1A .	5.3 s.u.
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	44 Report



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	7 Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	8 Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	2 Report
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.500 Check
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.003 Degree
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	1 Report
PLAT173_ALERT_4_G	The CIF-Embedded .res File Contains DANG Records	2 Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	2 Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	1 Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	2 Report
PLAT300_ALERT_4_G	Atom Site Occupancy of S1A Constrained at	0.87 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of S1B Constrained at	0.13 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O1A Constrained at	0.87 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O1B Constrained at	0.13 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C14A Constrained at	0.87 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C15A Constrained at	0.87 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C14B Constrained at	0.13 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C15B Constrained at	0.13 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H14A Constrained at	0.87 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H14B Constrained at	0.87 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H14C Constrained at	0.87 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H15A Constrained at	0.87 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H15B Constrained at	0.87 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H15C Constrained at	0.87 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H14D Constrained at	0.13 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H14E Constrained at	0.13 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H14F Constrained at	0.13 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H15D Constrained at	0.13 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H15E Constrained at	0.13 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H15F Constrained at	0.13 Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	14% Note
PLAT413_ALERT_2_G	Short Inter XH3 .. XHn H10A ..H15D .	1.98 Ang.
	x,-1+y,z =	1_545 Check
PLAT413_ALERT_2_G	Short Inter XH3 .. XHn H12C ..H15F .	2.11 Ang.
	2-x,1-y,1-z =	2_766 Check
PLAT431_ALERT_2_G	Short Inter HL..A Contact I1 ..O1 .	3.28 Ang.
	1-x,1-y,-z =	2_665 Check
PLAT431_ALERT_2_G	Short Inter HL..A Contact I1A ..O4 .	2.93 Ang.
	1+x,y,z =	1_655 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O2 ..C21A .	3.01 Ang.
	x,-1+y,z =	1_545 Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	16 Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	54 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	360	Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File		1	Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity		1.6	Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.		4	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
 43 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 10 ALERT type 2 Indicator that the structure model may be wrong or deficient
 5 ALERT type 3 Indicator that the structure quality may be low
 27 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.

