

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) kt-11a_a

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: kt-11a_a

Bond precision: C-C = 0.0104 Å Wavelength=0.71073

Cell: a=13.2480(4) b=13.2888(4) c=15.1807(5)
 alpha=96.352(1) beta=102.068(1) gamma=115.906(1)
Temperature: 150 K

	Calculated	Reported
Volume	2288.06(13)	2288.06(12)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	I28 Sb8, 4(C7 H10 N)	6(I3 Sb), 2(I4 Sb), 2(I), 4(C7 H10 N)
Sum formula	C28 H40 I28 N4 Sb8	C28 H40 I28 N4 Sb8
Mr	4959.92	4959.84
Dx, g cm ⁻³	3.600	3.600
Z	1	1
Mu (mm ⁻¹)	11.793	11.793
F000	2128.0	2128.0
F000'	2111.05	
h,k,lmax	17,17,20	17,17,20
Nref	11387	11320
Tmin,Tmax	0.573,0.702	0.528,0.746
Tmin'	0.304	

Correction method= # Reported T Limits: Tmin=0.528 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.994 Theta(max)= 28.302

R(reflections)= 0.0314(8945)	wR2(reflections)= 0.0535(11320)
S = 0.999	Npar= 380

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: I28 Sb8, 4(C7 H10 N)
Rep.: 6(I3 Sb), 2(I4 Sb), 2(I), 4(C7 H10 N)

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Sb4 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C6 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 4) 2.2 Note
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.0104 Ang.
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 7 Note
1 0 0, -1 1 0, 0 1 0, 0 -1 1, -1 0 1, 0 0 1,
-1 1 1,

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & Sth/L= 0.600 45 Report
-13 1 0, -4 1 0, 12 1 0, -15 7 0, 3 12 0, 15 -7 1,
-1 4 1, -15 7 1, 15 -7 2, 14 -4 2, -14 3 2, -15 7 2,
-14 3 3, -15 8 3, 14 -5 4, -13 -1 4, -13 0 4, -14 3 4,
1 -4 5, -13 0 5, -11 1 5, -14 3 5, -13 0 6, 6-14 7,
-13 0 7, -14 4 7, -14 5 7, 2-10 8, -4 10 10, 4-12 11,
5-12 11, 6-12 11, 7-12 11, 8-12 11, 1-11 12, 8-11 12,
-3 8 12, 0-10 13, 7-10 13, 1 -9 14, 2 -9 14, 3 -9 14,
7 -8 14, 3 -7 15, 4 -7 15,

PLAT977_ALERT_2_C Check Negative Difference Density on H3 . -0.33 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H9 . -0.39 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H10A . -0.33 eA-3



Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 9 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 2 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.001 Degree
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 4 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
PLAT231_ALERT_4_G Hirshfeld Test (Solvent) N1 --C6 . 8.0 s.u.
PLAT231_ALERT_4_G Hirshfeld Test (Solvent) C5 --C6 . 8.2 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) I4 --Sb1 . 11.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) I4 --Sb3_a . 10.7 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) I8 --Sb2 . 28.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) I8 --Sb2_a . 19.7 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) I10 --Sb4 . 11.0 s.u.
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
PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 3) 11.23 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 4) 6.77 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 3 Note
H8AA H8AB H8AC

PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 2 Note
C7 H10 N

PLAT794_ALERT_5_G Tentative Bond Valency for Sb1 (III) . 3.27 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Sb2 (III) . 3.12 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Sb3 (III) . 3.26 Info

PLAT794_ALERT_5_G	Tentative Bond Valency for Sb4	(III)	.	3.27	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		124	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary	.			Please Do !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600		15	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF		2	Note
	-4 1 0, -1 4 1,				
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File			1	Note
	0 1 0,				
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		2.3	Low
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value		1.14	Note
	Predicted wR2: Based on SigI**2	4.68	or SHELX Weight	5.45	
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
10 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
32 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
14 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
14 ALERT type 4 Improvement, methodology, query or suggestion
5 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 kt-11a_a - ellipsoid plot

