

# checkCIF/PLATON report

No syntax errors found.      CIF dictionary      Interpreting this report

## Datablock: I

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Bond precision:    N- C = 0.0225 A

Wavelength=0.71073

Cell:                a=10.8746(8)                b=11.2843(7)                c=15.0197(7)  
                              alpha=99.886(5)                beta=96.852(5)                gamma=94.714(5)

Temperature:    150 K

	Calculated	Reported
Volume	1792.8(2)	1792.81(19)
Space group	P -1	P -1
Hall group	-P 1	?
Moiety formula	C9 H18 N3 S6 Sb	?
Sum formula	C9 H18 N3 S6 Sb	C18 H36 N6 S12 Sb2
Mr	482.44	964.75
Dx,g cm-3	1.787	1.787
Z	4	2
Mu (mm-1)	2.228	2.228
F000	960.0	960.0
F000'	960.77	
h,k,lmax	12,13,17	12,13,17
Nref	6308	6292
Tmin,Tmax	0.624,0.732	0.628,0.746
Tmin'	0.593	

Correction method= MULTI-SCAN

Data completeness= 0.997

Theta(max)= 25.000

R(reflections)= 0.1432( 4452)

wR2(reflections)= 0.4007( 6292)

S = 1.422

Npar= 355

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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.

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### Alert level A

PLAT213\_ALERT\_2\_A Atom C4 has ADP max/min Ratio ..... 6.4 oblat

**Author Response:** The high variation in ADP max/min ratio of C4 caused by dynamic disorder or due to thermal motion. We have tried to resolve this disorder by assigning alternative positions, but atom continues to have high ADP max/min ratio.

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### Alert level B

DIFMX01\_ALERT\_2\_B The maximum difference density is > 0.1\*ZMAX\*1.00

\_refine\_diff\_density\_max given = 8.475

Test value = 5.100

RFACR01\_ALERT\_3\_B The value of the weighted R factor is > 0.35

Weighted R factor given 0.401

PLAT084\_ALERT\_3\_B High wR2 Value (i.e. > 0.25) ..... 0.40

PLAT097\_ALERT\_2\_B Large Reported Max. (Positive) Residual Density 8.48 eA-3

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### Alert level C

DIFMN02\_ALERT\_2\_C The minimum difference density is < -0.1\*ZMAX\*0.75

\_refine\_diff\_density\_min given = -4.808

Test value = -3.825

DIFMN03\_ALERT\_1\_C The minimum difference density is < -0.1\*ZMAX\*0.75

The relevant atom site should be identified.

DIFMX02\_ALERT\_1\_C The maximum difference density is > 0.1\*ZMAX\*0.75

The relevant atom site should be identified.

RFACG01\_ALERT\_3\_C The value of the R factor is > 0.10

R factor given 0.143

RINTA01\_ALERT\_3\_C The value of Rint is greater than 0.12

Rint given 0.137

PLAT020\_ALERT\_3\_C The value of Rint is greater than 0.12 ..... 0.137

PLAT048\_ALERT\_1\_C MoietyFormula Not Given ..... ? Do !

PLAT082\_ALERT\_2\_C High R1 Value ..... 0.14

PLAT098\_ALERT\_2\_C Large Reported Min. (Negative) Residual Density -4.81 eA-3

PLAT125\_ALERT\_4\_C No 'symmetry\_space\_group\_name\_Hall' Given ..... ? Do !

PLAT213\_ALERT\_2\_C Atom C11 has ADP max/min Ratio ..... 3.3 oblat

PLAT234\_ALERT\_4\_C Large Hirshfeld Difference S2 -- C1 .. 0.16 Ang.

PLAT234\_ALERT\_4\_C Large Hirshfeld Difference N1 -- C1 .. 0.16 Ang.

PLAT234\_ALERT\_4\_C Large Hirshfeld Difference S10 -- C11 .. 0.16 Ang.

PLAT234\_ALERT\_4\_C Large Hirshfeld Difference N5 -- C11 .. 0.16 Ang.

PLAT234\_ALERT\_4\_C Large Hirshfeld Difference N6 -- C12 .. 0.16 Ang.

PLAT234\_ALERT\_4\_C Large Hirshfeld Difference N6 -- C17 .. 0.19 Ang.

PLAT413\_ALERT\_2\_C Short Inter XH3 .. XHn H4B .. H9B .. 2.13 Ang.

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### Alert level G

PLAT005\_ALERT\_5\_G No \_iucr\_refine\_instructions\_details in the CIF ? Do !

PLAT045\_ALERT\_1\_G Calculated and Reported Z Differ by ..... 2.00 Ratio

PLAT072\_ALERT\_2\_G SHELXL First Parameter in WGHT Unusually Large. 0.20

PLAT154\_ALERT\_1\_G The su's on the Cell Angles are Equal ..... 0.00500 Deg.

PLAT764\_ALERT\_4\_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.11 Ratio

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- 1 **ALERT level A** = Most likely a serious problem - resolve or explain
- 4 **ALERT level B** = A potentially serious problem, consider carefully
- 18 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
- 5 **ALERT level G** = General information/check it is not something unexpected

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

9 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

8 ALERT type 4 Improvement, methodology, query or suggestion

1 ALERT type 5 Informative message, check

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# checkCIF publication errors

## Alert level A

PUBL012\_ALERT\_1\_A \_publ\_section\_abstract is missing.  
Abstract of paper in English.

## Alert level G

PUBL013\_ALERT\_1\_G The \_publ\_section\_comment (discussion of study) is missing. This is required for a full paper submission (but is optional for an electronic paper).

PUBL017\_ALERT\_1\_G The \_publ\_section\_references section is missing or empty.

- 1 **ALERT level A** = Data missing that is essential or data in wrong format
- 2 **ALERT level G** = General alerts. Data that may be required is missing

PLATON version of 01/06/2013; check.def file version of 24/05/2013

Datablock I - ellipsoid plot

