

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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: I

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Bond precision:	C-C = 0.0036 Å	Wavelength=0.71073
Cell:	a=8.2706(4)	b=8.7726(4)      c=13.6433(7)
	alpha=76.091(2)	beta=74.610(2)      gamma=87.970(2)
Temperature:	296 K	
	Calculated	Reported
Volume	925.98(8)	925.98(8)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C16 H13 Cl2 N3 O3 S2	C16 H13 Cl2 N3 O3 S2
Sum formula	C16 H13 Cl2 N3 O3 S2	C16 H13 Cl2 N3 O3 S2
Mr	430.31	430.31
Dx,g cm-3	1.543	1.543
Z	2	2
Mu (mm-1)	0.598	0.598
F000	440.0	440.0
F000'	441.24	
h,k,lmax	11,11,18	11,11,18
Nref	4627	4598
Tmin,Tmax	0.622,0.734	0.600,0.750
Tmin'	0.549	

Correction method= # Reported T Limits: Tmin=0.600 Tmax=0.750  
AbsCorr = MULTI-SCAN

Data completeness= 0.994      Theta(max)= 28.350

R(reflections)= 0.0561( 4134)      wR2(reflections)= 0.1554( 4598)

S = 1.030      Npar= 216

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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 C**

PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	6 Report
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .		2 Check

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● **Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite		9 Note
PLAT063_ALERT_4_G	Crystal Size Likely too Large for Beam Size ....		0.99 mm
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)		0.002 Degree
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records		6 Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records		10 Report
PLAT174_ALERT_4_G	The CIF-Embedded .res File Contains FLAT Records		1 Report
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C12 --C16 .		5.1 s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for S1 --C1 .		14.0 s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for S1A --C2 .		7.6 s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for S1A --C4 .		10.7 s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C1 --C3A .		13.0 s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C2 --C3 .		6.0 s.u.
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1 )		38% Note
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters		1 Info
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms ....		! Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....		14 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	23 Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...		6 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		12 Info

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

1 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  
4 ALERT type 3 Indicator that the structure quality may be low  
6 ALERT type 4 Improvement, methodology, query or suggestion  
1 ALERT type 5 Informative message, check

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## Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

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**PLATON version of 30/01/2018; check.def file version of 30/01/2018**

Datablock I - ellipsoid plot

