

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) t

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: t

Bond precision:	C-C = 0.0055 A	Wavelength=1.54178
Cell:	a=13.9963 (1) alpha=90	b=13.9963 (1) beta=90
		c=30.1665 (6) gamma=120
Temperature:	173 K	
	Calculated	Reported
Volume	5117.79 (13)	5117.78 (13)
Space group	P 61	P 61
Hall group	P 61	P 61
Moiety formula	C16 H26 O5 S	C16 H26 O5 S
Sum formula	C16 H26 O5 S	C16 H26 O5 S
Mr	330.43	330.43
Dx, g cm ⁻³	1.287	1.287
Z	12	12
Mu (mm ⁻¹)	1.863	1.863
F000	2136.0	2136.0
F000'	2146.24	
h, k, lmax	16, 16, 36	16, 16, 36
Nref	6254 [3191]	6250
Tmin, Tmax	0.779, 0.800	0.602, 0.753
Tmin'	0.707	

Correction method= # Reported T Limits: Tmin=0.602 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 1.96/1.00 Theta (max)= 68.266

R(reflections)= 0.0317 (5717)	wR2(reflections)= 0.0883 (6250)
S = 0.947	Npar= 442

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

PLAT089_ALERT_3_C	Poor Data / Parameter Ratio (Zmax < 18)	7.22	Note
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	3.1	Ratio
PLAT220_ALERT_2_C	NonSolvent Resd 2 C Ueq(max)/Ueq(min) Range	3.2	Ratio
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C7	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C24	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C8	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C25	Check
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00546	Ang.
PLAT413_ALERT_2_C	Short Inter XH3 .. XHn H36 ..H43 .	2.06	Ang.
	1+y,1-x+y,-1/6+z =	3_664	Check
PLAT767_ALERT_4_C	INS Embedded LIST 6 Instruction Should be LIST 4		Please Check
PLAT767_ALERT_4_C	INS Embedded LIST 6 Instruction Should be LIST 4		Please Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	3	Report
PLAT987_ALERT_1_C	The Flack x is >> 0 - Do a BASF/TWIN Refinement		Please Check



Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	2	Report
PLAT033_ALERT_4_G	Flack x Value Deviates > 3.0 * sigma from Zero .	0.024	Note
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem	2	100 %Fit
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem	2	100 %Fit
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem	2	100 %Fit
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem	2	100 %Fit
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem	2	100 %Fit
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem	2	100 %Fit
PLAT113_ALERT_2_G	ADDSYM Suggests Possible Pseudo/New Space Group	P6122	Check
	Check Model Parameter Symmetry for Reflection Data Support		
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 1)	5% Note
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 2)	5% Note
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H6 ..H9BB .	2.08	Ang.
	x,y,z =	1_555	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H13 ..H9BA .	1.90	Ang.
	x,y,z =	1_555	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H26A ..H35 .	2.03	Ang.
	x,y,z =	1_555	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H26C ..H43 .	2.04	Ang.
	x,y,z =	1_555	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	6	Note
PLAT791_ALERT_4_G	Model has Chirality at C2 (Sohnke SpGr)		S Verify
PLAT791_ALERT_4_G	Model has Chirality at C3 (Sohnke SpGr)		R Verify
PLAT791_ALERT_4_G	Model has Chirality at C4 (Sohnke SpGr)		R Verify
PLAT791_ALERT_4_G	Model has Chirality at C5 (Sohnke SpGr)		S Verify
PLAT791_ALERT_4_G	Model has Chirality at C12 (Sohnke SpGr)		R Verify
PLAT791_ALERT_4_G	Model has Chirality at C19 (Sohnke SpGr)		S Verify
PLAT791_ALERT_4_G	Model has Chirality at C20 (Sohnke SpGr)		R Verify
PLAT791_ALERT_4_G	Model has Chirality at C21 (Sohnke SpGr)		R Verify
PLAT791_ALERT_4_G	Model has Chirality at C22 (Sohnke SpGr)		S Verify
PLAT791_ALERT_4_G	Model has Chirality at C30 (Sohnke SpGr)		R Verify
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	2	Note

PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	1 Note
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged	Please Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	14 Info

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
21 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
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.

Datablock t - ellipsoid plot

