

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

Bond precision:	C-C = 0.0060 A	Wavelength=1.54180	
Cell:	a=6.9914 (3)	b=14.1455 (7)	c=27.1767 (11)
	alpha=90	beta=90	gamma=90
Temperature:	173 K		
	Calculated	Reported	
Volume	2687.7 (2)	2687.7 (2)	
Space group	P 21 21 21	P 21 21 21	
Hall group	P 2ac 2ab	P 2ac 2ab	
Moiety formula	C18 H21 N O3, C12 H14 N2 O3	C18 H21 N O3, C12 H14 N2 O3	
Sum formula	C30 H35 N3 O6	C30 H35 N3 O6	
Mr	533.61	533.61	
Dx, g cm ⁻³	1.319	1.319	
Z	4	4	
Mu (mm ⁻¹)	0.753	0.753	
F000	1136.0	1136.0	
F000'	1139.55		
h, k, lmax	8, 16, 32	8, 16, 32	
Nref	4786 [2755]	4466	
Tmin, Tmax	0.956, 0.963	0.680, 1.000	
Tmin'	0.860		

Correction method= # Reported T Limits: Tmin=0.680 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.62/0.93 Theta (max)= 66.846

R(reflections)= 0.0500 (3560) wR2(reflections)=
S = 1.027 Npar= 404 0.1289 (4466)

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**

STRVA01_ALERT_4_C	Flack parameter is too small		
	From the CIF: <code>_refine_ls_abs_structure_Flack</code>	-0.300	
	From the CIF: <code>_refine_ls_abs_structure_Flack_su</code>	0.300	
PLAT018_ALERT_1_C	<code>_diffn_measured_fraction_theta_max</code>	.NE. *_full	! Check
PLAT089_ALERT_3_C	Poor Data / Parameter Ratio (Zmax < 18)	6.77 Note
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00596 Ang.
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.596	18 Report

● **Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite		15 Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...		9 Report
PLAT032_ALERT_4_G	Std. Uncertainty on Flack Parameter Value High	. 0.300	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records		4 Report
PLAT175_ALERT_4_G	The CIF-Embedded .res File Contains SAME Records		1 Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records		2 Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records		1 Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used		0.0100 Report
PLAT189_ALERT_3_G	A Non-default SAME Restraint Value for First Par		0.0100 Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used		0.0100 Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used		0.0100 Report
PLAT300_ALERT_4_G	Atom Site Occupancy of C11B	Constrained at	0.65 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C12B	Constrained at	0.65 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C13B	Constrained at	0.65 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C14B	Constrained at	0.65 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C11C	Constrained at	0.35 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C12C	Constrained at	0.35 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C13C	Constrained at	0.35 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C14C	Constrained at	0.35 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H10C	Constrained at	0.65 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H11B	Constrained at	0.65 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12B	Constrained at	0.65 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H13A	Constrained at	0.65 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H13B	Constrained at	0.65 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H14B	Constrained at	0.65 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H14C	Constrained at	0.65 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H10D	Constrained at	0.35 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H11C	Constrained at	0.35 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12C	Constrained at	0.35 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H13C	Constrained at	0.35 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H13D	Constrained at	0.35 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H14D	Constrained at	0.35 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H14E	Constrained at	0.35 Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)		24% Note
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O3A	.	107.3 Degree
PLAT480_ALERT_4_G	Long H...A H-Bond Reported H17C	..02B	2.64 Ang.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	5 Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	133 Note
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max)	Still	59% Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		1 Note

PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	3	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.4	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
5 **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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
11 ALERT type 3 Indicator that the structure quality may be low
31 ALERT type 4 Improvement, methodology, query or suggestion
0 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.

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